NANOTECH FRANCE 2022

Biotech
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GAMS
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15 - 17 June 2022, Paris , France

Book of Abstracts

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Nanotech France 2022 / NanoMatEn 2022 / NanoMetrology 2022 / GAMS 2022 / Biotech France 2022
Joint Conferences Preliminary Program
15 - 17 June 2022, Paris, France

June 15, 2022		
08:00 - 12:00	**Onsite Participant registration**	
Nanotech / GAMS Joint Plenary session		
Amphithéâtre		
Session's Chairs: **Prof. Jacques Jupille, Institut des Nanosciences de Paris, France** **Dr. Arantzazu Garcia-Lekue, Donostia International Physics Center, Spain** **Prof. Rodrigo Ferrão de Paiva Martins, Nova Univ. of Lisbon, Portugal**		
10:00 - 10:30	Using 2D materials in a 3-dimensional world: from nanochemistry to technology applications **V. Palermo**	**Prof. Vincenzo Palermo,** Institute for Organic Synthesis and Photoreactivity- CNR - **Italy**
10:30 - 11:00	LEGO chemistry for graphene-based nanoarchitectures: from 0D quantum dots to 2D lateral heterostructures **A. Mugarza**	**Prof. Aitor Mugarza,** Catalan Institute of Nanoscience and Nanotechnology (ICN2), **Spain**
11:00 - 11:30	0D + 1D = 2D: Heterogeneous Electrodes by Electrospinning Q. Li, F. Yan and **J. Texter**	**Prof. John Texter**, Eastern Michigan University, **USA**
11:30 - 12:00	Modelling complex nanosystems for drug delivery, targeting and imaging **C. Di Valentin**	**Prof. Cristiana Di Valentin,** University of Milan-Bicocca, **Italy**
12:00 - 12:30	Synthesis of (multi-)Metal core-shell and alloyed nanoparticles by atmospheric pressure plasma filament-surface interaction **J-P. Borra**	**Prof. Jean-Pascal Borra**, Paris-Saclay University, **France**
12:00 - 14:00	**Lunch Break**	
Nanotech / GAMS Joint Session I.A: **Nanomaterials Fabrication / Synthesis / properties**		
Amphithéâtre		
Session's Chairs: **Prof. Jacques Jupille, Institut des Nanosciences de Paris, France** **Prof. John Texter, Eastern Michigan University, USA** **Prof. Jean-Pascal Borra, Paris-Saclay University, France**		
14:00 - 14:30	Addressing magnetic and topological properties of graphene nanoribbons **A. Garcia-Lekue**	**Dr. Arantzazu Garcia-Lekue**, Donostia International Physics Center, **Spain**
14:30 - 15:00	Growth of transition metal dichalcogenides on sapphire by Molecular beam epitaxy. Application to high frequency detectors and mixers **P. Legagneux**	**Dr. Pierre Legagneux**, Thales Research and Technology- Palaiseau, **France**
15:00 - 15:15	One-step Elaboration of Janus Polymeric Nanoparticles **M. Vauthier** and C. A. Serra	**Dr. Madeline Vauthier**, University of Strasbourg, **France**
15:15- 15:30	Calix[4]arene-Tetradiazonium Salts: a Powerful and Versatile Tool for Nanomaterials Functionalization. M. Retout, B. Gosselin, I. Jabin and **G. Bruylants**	**Prof. Gilles Bruylants**, Université libre de Bruxelles, **Belgium**
15:30 - 15:45	Mass producing of TEMPO oxidized nanofibers from thermomecanical pulp for various applications: global approach needed D. Myja, **E. Loranger** and R. Lanouette	**Prof Eric Loranger,** University of Quebec in Trois-Rivières, **Canada**

15:45 - 16:00	Synthesis, characterization and industrial application of a nanofluid based on copper nanoparticles with long-lasting antimicrobial effect **E. Salas-Huenuleo**, R. Torres, N. Wainstein, O. Oviedo-Rojas, L. Salas-Huenuleo and P. Valenzue-la-Bustamante	**Mr. Edison Salas-Huenuleo**, Advanced Integrated Technologies, **Chile**
16:00 - 16:30	**Afternoon Coffee Break**	
Session's Chairs: **Prof. John Texter, Eastern Michigan University, USA** **Dr. Pierre Legagneux, Thales Research and Technology- Palaiseau, France.** **Prof. Jean-Pascal Borra, Paris-Saclay University, France**		
16:30 - 17:00	Electro-Flexure Response of Multi-Functional Natural Fiber Hybrid Composites C. Meninno, V. Chalivendra and **Y. Kim**	**Prof. Yong K Kim**, Univ. of Maaaschusetts Dartmouth, **USA**
17:00 - 17:15	Synthesis of porous high-temperature superconductors via a templated approach **E. Luke**, J. Potticary, L. Terry, H. Doan, V. Ting, S. Friedemann and S.R Hall	**Ms. Emily Luke**, University of Bristol, **UK**
17:15 - 17:30	From solution to surface: Molecular engineering of functional supra-molecular assemblies on graphene-based surfaces **S. Moradmand,** Q. Fernez, O. De Luca, L. Sosa Vargas, P. Rudolf and I. Arfaoui	**Ms. Shiva Moradmand**, Sorbonne University, **France**
17:30 - 17:45	Ionic concentration and substrate dependent surface potential of single layer graphene by in-liquid Dual-Harmonic KPFM **M. Delgà-Fernández**, E. del Corro, L. Collins, M. Checa, X. Illa, A. P. Pérez and J. A. Garrido	**Mrs. Marta Delga Fernandez**, Catalan Institute of Nanoscience and Nanotechnology, **Spain**
17:45 - 18:00	Submicron 4D Printing of Shape Memory Polymer **W. Zhang**, H. Wang, H.T. Wang and J.K.W. Yang	**Mr. Wang Zhang**, Singapore University of Technology and Design, **Singapore**
18:00 - 18:15	3D Printed Colorful Vortex Beam Generator and Decoder **H. Wang**, H. Wang, W. Zhang, J.Y.E. Chan and J. K.W. Yang	**Mr. Hongtao Wang**, Singapore University of Technology and Design, **Singapore**
18:15 - 18:30	Nanoscale 3D Printing of Light Field Prints **J.Y.E. Chan**, Q. Ruan, M. Jiang, H. Wang, H. Wang, W. Zhang, C-W. Qiu and J.K.W. Yang	**Mr. John Chan,** Singapore University of Technology and Design, **Singapore.**
18:30 - 18:45	Effect of Nano Silica on Mechanical and Water absorption properties of Hybrid composites of Basalt fibers, Glass fibers, Hemp fibers and Unsaturated Polyester Resin P. Dayalan and **P.A Mahanwar**	**Prof. Prakash Mahanwar**, Institute of Chemical Technology- Mumbai, **India**
18:45 – 19:00	The investigation of cathode layer of Molten Carbonate Fuel Cell manufactured by using printing techniques **J. Milewski**	**Prof. Jaroslaw Milewski**, Warsaw University of Technology, **Poland**

June 15, 2022		
Nanotech / NanoMetrolgy joint session I.B: **Nanomaterials Modelling and Characterisation**		
Conference Room Derain 1+2		
Session's Chairs: **Prof. Yong K Kim, Univ. of Maaaschusetts Dartmouth, USA** **Prof. Vincenzo Palermo, Institute for Organic Synthesis and Photoreactivity- CNR, Italy** **Prof. Aitor Mugarza, Catalan Institute of Nanoscience and Nanotechnology (ICN2), Spain**		
14:00 - 14:30	TEM and related microanalytical techniques: a powerful tool for the characterization of low band-gap rod-coil block copolymer:PC61BM blend water-processable nanoparticles **A.M.Ferretti** and S.Zappia	**Dr. Anna Maria Ferretti**, CNR-SCITEC Milano, **Italy**
14:30 - 15:00	Ethics of Nanotechnology in the framework of the NanoFabNet Hub for sustainable, industrial-scale Nanofabrication **F. Doridot**	**Dr. Fernand Doridot**, Center for Ethics, Technics and Society, **France**
15:00 - 15:15	Length and diameter determination of rod-like nanoparticles using Depolarized Dynamic Light Scattering **B. Maxit**, F.Aubrit, H. Anop, S. Boj, O. Sandre and D. Jacob	**Dr. Benoit Maxit,** Cordouan Technologies, **France**
15:15 - 15:30	A Unique And Enhanced Approach To Measure The Effective Surface Tension of A nanoparticle coated Liquid Marble **P. Singha**, N-K. Nguyen, J. Zhang, N-T. Nguyen and C. H. Ooi	**Mr. Pradip Singha**, Griffith University, **Australia**
15:30 - 15:45	Experimental characterization and numerical modelling of polymer-based nanocomposite properties **G. Ongaro**, R. Bertani, U. Galvanetto and M. Zaccariotto	**Mrs. Greta Ongaro**, University of Padova, **Italy**
15:45 - 16:00	Quantification of the Total and Accessible Number of Functional Groups and Ligands on Nanomaterials **I. Tavernaro**, N. Nirmalananthan-Budau and U. Resch-Genger	**Dr. Isabella Tavernaro**, BAM- Berlin, **Germany**
16:00 - 16:30	**Afternoon Coffee Break**	
Session's Chairs: **Dr. Fernand Doridot, Center for Ethics, Technics and Society, France** **Dr. Anna Maria Ferretti, CNR-SCITEC Milano, Italy**		
16:30 - 16:45	Microfluidics and Microscopy – A Powerful Combination for the Development of Novel Micro-and Nano-structured Soft Materials with Designer Functionality **C. Hao**, D. Scholz, N. Stephens and G. Redmond	**Ms. Chenxi Hao**, University College Dublin, Dublin, Ireland
16:45 - 17:00	Physico-Chemical Characterization of Hydroxyapatite Nanoparticles from Tricalcium Phosphate Food Additive **Y. El Moussaoui**, H. Terrisse, S. Quillard, MH. Ropers and B. Humbert	**Mr. Youssef El Moussaoui,** Nantes University, **France**
17:00 - 17:15	A simple approach to the deflection detection of the nanowires **M. Sharma**, A.S. Prasad, B. Büchner and T. Mühl	**Ms. Maneesha Sharma,** TU Dresden, **Germany**
17:15 - 17:30	Iron Oxide Nanoparticles as Versatile Nanoscale Reference Materials **S.-L. Abram**, P. Mrkwitschka, A. F. Thünemann, B. Rühle, O. Löhmann, P. Kuchenbecker, H. Bresch, V.-D. Hodoroaba, and U. Resch-Genger	**Dr. Sarah-Luise Abram**, Federal Institute for Materials Research and Testing, **Germany**
17:30 - 17:45	Tiered Approach Strategy for Occupational Risk Assessment and Management of Lightweight Metals Reinforced with Nanomaterials using Direct Energy Deposition Process **J. Laranjeira**, C. Matos, A. R. Alberto, C. F. Martins, K. F. Neves and M. F. N. N. Carvalho	**Dr. João Laranjeira**, ISQ Institute, **Portugal**
17:45 - 18:00	The monitoring system of nanoaerosols and noise hazards in an industrial facility based on low-cost environmental sensors **T. Jankowski** and P. Sobiech	**Dr. Tomasz Jankowski**, Central Institute for Labour Protection, **Poland**

June 15, 2022		
Biotech Session I. A		
Conference Room Moreau 1		
Session's Chairs: **Prof. Magali Remaud-Simeon, INSA Toulouse, France** **Prof. Izabela Michalak, Wroclaw University of Science and Technology, Poland** **Prof. Khaled Masmoudi, United Arab Emirates, UAE**		
11:00 - 11:30	Laboratory digitalization and automation – the challenges of faster bioprocess development **P. Neubauer** and M. N. Cruz Bournazou	**Prof. Peter Neubauer**, Technische Universitat Berlin, **Germany**
11:30 - 12:00	The autotrophic metabolism as interface between renewable energy and redox biocatalysis. **R. Kourist**	**Prof. Robert Kourist**, Graz University of Techology, **Austria**
12:00 - 14:00	**Lunch Break**	
Session's Chairs: **Prof. Peter Neubauer, Technische Universitat Berlin, Germany** **Prof. Saulius Klimasauskas, Vilnius University, Lithuania**		
14:00 - 14:30	An enzymatic journey into glycopolymer country **M. Remaud-Simeon**	**Prof. Magali Remaud-Simeon**, INSA Toulouse, **France**
14:30 - 15:00	Process engineering strategies towards efficient biocatalytic processes **S. Kara**	**Prof. Selin Kara**, Aarhus Univ., **Denmark &** Leibniz Univ. Hannover, **Germany**
15:00 - 15:15	Photobiocatalytic Oxyfunctionalization with High Reaction Rate using a Baeyer-Villiger Monooxygenase from Burkholderia xenovorans in Metabolically Engineered Cyanobacteria **L. Malihan-Yap**, E. Erdem, L. Assil-Companioni, H. Grimm, G. Barone, C. Serveau-Avesque, A. Amouric, K. Duquesne, V. Berardinis, Y. Allahverdiyeva, V. Alphand and R. Kourist	**Dr. Lenny Malihan-Yap**, Graz University of Technology, **Austria**
15:15 - 15:30	Biocatalytic synthesis of novel polyesteramide nanoparticles derived from ε-caprolactam and hydroxy acids **I.C. Benea**, D.M. Dreavă, I. Bîtcan, C. Paul, A. Todea, L. Nagy, S. Kéki, I. Kántor , T. Feczkó and F. Péter	**Ms. Ioana-Cristina Benea**, Politehnica University Timisoara, **Romania**
15:30 - 15:45	Seed Oilcakes Biorefinery as a Promising Renewable Resources for Producing Value-Added Products **S. F. Mirpoor**, C.V. L. Giosafatto and R.Porta	**Ms. Seyedeh.F. Mirpoor**, Federico II University of Naples, **Italy**
15:45 - 16:00	Green seaweed – Enteromorpha sp. as a feedstock for bioprocess engineering N. Niedzbała, E. Lorenc-Grabowska, P. Rutkowski, A. Szymczycha-Madeja, M. Wełna and **I. Michalak**	**Prof. Izabela Michalak**, Wroclaw University of Science and Technology, **Poland**
16:00 - 16:30	**Afternoon Coffee Break**	
Session's Chairs: **Prof. Izabela Michalak, Wroclaw University of Science and Technology, Poland** **Prof. Khaled Masmoudi, United Arab Emirates, UAE**		
16:30 - 16:45	Engineering Methyltransferase Pathways for Selective Chemical Tracking of Epigenetic Writers in Mammalian Cells V. Stankevičius, P. Gibas, B. Masiulionytė, L. Gasiulė, V. Masevičius, G. Vilkaitis and **S. Klimašauskas**	**Prof. Saulius Klimasauskas**, Vilnius University, **Lithuania**
16:45 - 17:00	Evolution-guided metabolic engineering for improving synthetic, genome-reduced co-cultures of C. glutamicum **S. Schito**, R. Zuchowski, F. Neuheuser, M. Bott, W. Wiechert, M. Baumgart and S. Noack	**Mr. Simone Schito**, Jülich Research Centre, **Germany**
17:00 - 17:15	What if Escherichia coli fails? Exploiting an Antarctic bacterium for the production of proteins harbouring intrinsically disordered regions **A. Colarusso**, C. Lauro, M. Calvanese, E. Parrilli and M.L. Tutino	**Dr. Concetta Lauro**, Federico II University of Naples, **Italy**

17:15 - 17:30	Membrane transporter identification and modulation via adaptive laboratory evolution **M.Radi** and A. Feist	**Mr. Mohammad Radi**, Technical University of Denmark, **Denmark**
17:30 - 17:45	Engineering Escherichia coli to produce industrially relevant oleochemicals **P. Matthay**, K. Bernaerts, K. Simoens, N. Verstraeten and J. Michiels	**Mr. Paul Matthay**, KU Leuven, **Belgium**
17:45 - 18:00	Microencapsulation of primary human tonsillar B cells for directed ex vivo cultivation platform **S. B. Huang**, M. Helm, V. Jérôme and R. Freitag	**Mr. Songyan Ben Huang**, University of Bayreuth, **Germany**
18:00 - 18:15	Multifaceted Roles of Versatile LEA-II Proteins from Cereals and Date Palm **K. Masmoudi**, M. Abdul Aziz, S. Rahman and F. Brini	**Prof. Khaled Masmoudi**, United Arab Emirates, **UAE**
18:15 - 18:30	The Ethics of synthetic meat. Hypes and hopes of a new challenging technology **L. Lo Sapio**	**Mr. Luca Lo Sapio**, The University of Turin, **Italy**

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Nanotech / GAMS / Biotech Joint session II.

Amphithéâtre

Session's Chairs:
Prof. Saulius Klimasauskas, Vilnius University, Lithuania
Prof. Magali Remaud-Simeon, INSA Toulouse, France

08:30 - 09:00	Making the enzymatic synthesis of bio-based polyesters feasible: from bioinformatics to pilot plant A. Todea, F. Asaro, M. Spennato, F. Zappaterra and **L.Gardossi**	**Prof. Lucia Gardossi**, University of Trieste, **Italy**
09:00 - 09:15	Use of a Microbioreactor for Screening of Fungal/Bacterial Co-culture Activity against a Fusarium Strain **E. Mephane**, E. Heuson, N. Imatoukene, M. Lopez and V. Phalip	**Ms. Eléonore Mephane**, Univ. Lille, **France**
09:15 - 09:30	Stereoselective synthesis of whisky lactones catalysed by bacteria from Rhodococcus erythropolis species **D. Hernik**, F. Boratyński and E. Brenna	**Mr. Dawid Hernik**, Wroclaw University of Environmental and Life Sciences, **Poland**
09:30 - 09:45	Fungistatic potential of Apiaceae lactones and their derivatives **J. Gach** and T. Olejniczak	**Ms. Joanna Gach**, Wrocław University of Environmental and Life Sciences, **Poland**
09:45 - 10:00	Effect of acid pretreatment on the primary products of biomass fast pyrolysis **D.O Usino**, T. Sar, P. Ylitervo and T. Richards	**Mr. David Usino**, University of Borås, **Sweden**
10:00 - 10:15	Much More than Salts and Mixtures: Functionalized Ionic Liquids and Eutectic Systems for Biomolecules Purification, Greenhouse F-gases Separation, and Drug Formulation S.F. Carvalho, J.C. Bastos, M.F. Ferreira, J. E. Sosa, P.J. Castro, A.B. Pereiro and **J.M. M. Araújo**	**Dr. João Araújo**, NOVA University Lisbon, **Portugal**
10:15 - 10:30	Bioprivileged Fluorinated Ionic Liquids in the Purification of Proteins: Towards Enhanced Tunability of Aqueous Biphasic Systems **S.F. Carvalho,** M.H. Custódio, A.B. Pereiro and J.M. M. Araújo	**Ms Sara Carvalho,** NOVA University Lisbon, **Portugal**
10:30- 10:45	Characterization and Biotechnological Potential of Extracellular Polysaccharides Synthesized by Alteromonas Strains Isolated from French Polynesia Marine Environments **P. Concórdio-Reis**, V. D. Alves, J. R. Pereira, X. Moppert, J. Guezennéc, M. A. M. Reis and F. Freitas	**Ms. Patrícia Concórdio-Reis**, NOVA University Lisbon, Caparica, **Portugal**

10:30 - 11:00 **Morning Coffee Break**

Session's Chairs:
Prof. Wolfgang Ensinger, Technical University Darmstadt, Germany

11:00 - 11:30	Nano(Bio)Technological approaches for the diagnosis of infectious diseases **M. P. Marco**	**Prof. Pilar Marco**, IQAC-CSIC/CIBER-BBN, **Spain**
11:30 - 12:00	Neurological phenotypic nanomedicines: BBB crossing and new therapy development **G. Battaglia**	**Prof. Giuseppe Battaglia,** ICREA/ IBEC/ BIST, Spain and University College London, **UK**
12:00 - 12:15	Advanced Dynamic Light Scattering and its Application to Life Sciences **C. Bretz,** A. Vaccaro and D. Leumann	**Dr. Coline Bretz**, LS Instruments, **Switzerland**

12:00 - 14:00 **Lunch Break**

June 16, 2022

Nanotech / Biotech - Session II.D:
Nanotechnology for life science- Biosensors, Diagnostics and Imaging

Amphithéâtre

Session's Chairs:
Prof. Pilar Marco, IQAC-CSIC/CIBER-BBN, Spain
Prof. Vincenzo Palermo, Institute for Organic Synthesis and Photoreactivity- CNR, Italy

14:00 - 14:30	Single Polymeric Ion-Conducting Nanochannels as Core of Biomolecular Sensors for Medical Diagnostics **W. Ensinger**	**Prof. Wolfgang Ensinger**, Technical University Darmstadt, **Germany**
14:30 - 14:45	WELFA : WAINVAM-E Lateral Flow Assay - Innovative and Ultra Sensitive LFA System using the Properties of NV Center Diamonds A. Bournigault-Nuquet, **D. Rani**, M. Raude, B. Shevchenko, R. Geiger	**Mrs. Ditpi Rani**, WAINVAM-E, **France**
14:45 - 15:00	Development of a novel carbonized porous silicon electrochemical sensing platform by pyrolysis of furfuryl alcohol **A.A. Rajendran**, K. Guo, M. Bujaldon Velasco, K. Shafique, P. Formentín, H. Haji-Hashemi, N.H. Voelcker, X. Cetó and B. Prieto-Simón	**Mr. Anandapadmanabhan A. Rajendran**, University of Rovira i Virgili, **Spain**
15:00- 15:15	Rapid fabrication of responsive biodegradable microstructures; an introduction to a low invasive research track of multiphoton polymerization for a resolved clinical application **A. Zeynali**, M. Budimir, M. Marini, M. Collini, M. Lecchi, S. Blasa and G. Chirico	**Dr. Amirbahador Zeynali**, University of Milano-Bicocca, **Italy**
15:15 - 15:30	in-vitro Monitoring of Extracellular Matrix Protein Conformations us-ing Gold-Edge-Coated Triangular Silver Nanoplates within a Cellular High-Noise Environment in the Presence of Chitosan Biocompatible Hydrogels **L.G. Rodriguez Barroso**, F. Azaman, R. Pogue, D. Devine and M. Brennan-Fournet	**Ms. Laura G. Rodriguez Barroso**, Technological University of the Shannon, **Ireland**
15:30 - 15:45	Self-Assembly of Carbohydrate-based Bottlebrushes in Solution: Glyco-Nanoparticles **H. Li** and R. Borsali	**Mr. Hong Li**, CERMAV-Univ. Grenoble Alpes, **France**
15:45 - 16:00	Probing the glycans accessibility of the nanoparticle biomolecular corona **E. Clemente**, M. Martinez-Moro, D. Spencer, R.A Gardner, M. Kotsias, S. Moya and M.P Monopoli	**Ms. Eva Clemente**, Royal College of Surgeons in Ireland, **Ireland**
16:00 - 16:30	**Afternoon Coffee Break**	
16:30 - 16:45	Gold nanoparticles long-term evaluation in liver: role of shape, size and surface functionalization **J. Fernandez Alarcon**, M. Soliman, T. Ludtke, E. Clemente, M. B. Violatto, A. Corbelli, F. Fiordaliso, C. Cordiglieri, L. Talamini, G. Sitia, S. Moya, P. Bigini and M. P. Monopoli	**Mrs. Jennifer Fernandez Alarcon**, The Mario Negri Institute for Pharmacological Research, **Italy**
16:45 - 17:00	Exploring the Synthesis Conditions for Magnetic Pd/Fe-oxide Nanoparticles **A. Maier**, R. van Oossanen, G. van Rhoon, A. G. Denkova and K. Djanashvili	**Ms. Alexandra Maier**, Delft University of Technology, **The Netherlands**
17:00 - 17:15	Polyhydroxyalkanoates (PHAs) and FucoPol based scaffolds for tissue engineering applications **J.R. Pereira**, A.M. Rafael, A. Esmail, P. Zoio, F. Silva, A.C. Marques4, C. Sevrin, C. Grandfils, E. Fortunato, A. Oliva, M.A. M. Reis and F. Freitas	**Mr. João Ricardo Pereira**, NOVA University Lisbon, **Portugal**

June 16, 2022

NanoMatEn / GAMS Joint Session III.A: Materials and Nanomaterials for Energy / Nanoelectronics/ Nanophotonics

Conference Room Derain 1+2

Session's Chairs:
Prof. Elisabetta Dimaggio, University of Pisa, Italy
Prof. Beongki Cho, Gwangju Institute of Science and Technology, Rep. of Korea
Prof. HyunChul Sohn, Yonsei University, Rep of Korea

08:30 - 09:00	Chipless Electronics: a Sustainable Commitment beyond Silicon **R. F. de Paiva Martins**	**Prof. Rodrigo Ferrão de Paiva Martins**, Nova Univ. of Lisbon, **Portugal**
09:00 - 09:30	Structural color in ordered and disordered photonic media **M. Eich**	**Prof Manfred Eich**, Hamburg University of Technology, **Germany**
09:30 - 10:00	Nanomaterials for Hydrogen, Fuel Cells and Thermal Energy **J.W. Sheffield**	**Prof. John W. Sheffield**, Purdue University, **USA**
10:00 - 10:15	Correlating the functional properties of graphene on the nanoscale I.M. Hermes, S. Krotkus, M. Heuken, B. Conran, **A. Klasen**, C. McAleese, X. Wang and O. Whear	**Dr. Alexander Klasen**, Park Systems Europe, **Germany**
10:15 - 10:30	Exploring Memristive Squaraine Microtubes: Programmable Multi-Level Memory Behaviour for Neuromorphic Applications **K. Griffin**	**Mr. Karl Griffin**, University College Dublin, **Ireland**
10:30 - 11:00	**Morning Coffee Break**	
11:00 - 11:15	Parametric spinwave excitation and mode control using built-in current in a NiFe nanowire **B. K. Cho**, S. H. Han and S. Hwang	**Prof. Beongki Cho**, Gwangju Institute of Science and Technology, **Rep. of Korea**
11:15 - 11:30	Nonlinear optical thermometry based on Upconversion Luminescence and Second Harmonic Generation (SHG) **T. Zheng**, M. Runowski, S. Lis, I.R. Martín, M. Vega and J. Llanos	**Mr. Teng Zheng**, Adam Mickiewicz University, **Poland**
11:30 - 11:45	Synthesis of tunable nano-lamellar transition metal hybrid materials and their behavior as battery electrode materials. **T. Riant**, J. Maynadie, and D. Meyer	**Mr. Tennessee Riant**, University of Montpellier, **France**
11:45 - 12:00	InN on Si(100) photovoltaic devices with an amorphous Si interlayer deposited by DC and RF sputtering **M. Sun**, F. B. Naranjo and S. Valdueza-Felip	**Mr. Michael Sun**, University of Alcala, **Spain**.
12:00 - 12:15	Trichalcogenide materials for small bandgap photovoltaic devices **E. Edri**	**Dr. Eran Edri**, Ben-Gurion University of the Negev, **Israel**
12:15 - 12:30	2D Organic-inorganic perovskites for next generation optoelectronics **K.J Riisnaes**, R. Mastia, A. Bacon, H.T Lam, L De Marco, M. Craciun and S. Russo	**Mr. Karl Jonas Riisnaes**, University of Exeter, **UK**
12:30 - 12:45	Photoexcitation dynamics and long-lived excitons in strain-engineered transition metal dichalcogenides N. Mondal, N. Azam, Y.N. Gartstein, M. Mahjouri-Samani and **A.V. Malko**	**Prof. Anton V. Malko**, The University of Texas at Dallas, **USA**
12:00 - 14:00	**Lunch Break**	

June 16, 2022		
NanoMatEn - Session III.B **Nanotechnology for Energy / Nanocatalysis (Part I)**		
Session's Chairs: **Prof. Rodrigo Ferrão de Paiva Martins, Nova Univ. of Lisbon, Portugal** **Prof Manfred Eich, Hamburg University of Technology, Germany**		
14:00 - 14:30	Boosting 2D semiconductors with molecules: high performance multi-responsive electronic devices **P. Samori**	**Prof. Paolo Samori**, University of Strasbourg, **France**
14:30 - 15:00	From classic technologies for novel devices, to novel approaches for classic devices **E. Dimaggio**	**Prof. Elisabetta Dimaggio**, University of Pisa, **Italy**
15:00 - 15:30	Nanoarchitecture for energy conversion **S. Christiansen**	**Prof. Silke Christiansen**, Fraunhofer IKTS, **Germany**
15:30 - 15:45	Bio-Inspired Materials for the Energy Challenge of the Century T. Tajima and **T. Massard**	**Dr. Thierry Massard**, AE Technologies, **USA**
15:45 - 16:00	Tuning the properties of 2D perovskites **A. Coriolano**, L.Polimeno, M. De Giorgi, D. Sanvitto and L. De Marco	**Mrs. Annalisa Coriolano**, University of Salento, **Italy**
16:00 - 16:30	**Afternoon Coffee Break**	
Session's Chairs: **Prof. Rodrigo Ferrão de Paiva Martins, Nova Univ. of Lisbon, Portugal** **Prof. John Texter, Eastern Michigan University, USA**		
16:30 - 16:45	Mott-insulator titanium sesquioxide: A novel electrochemical capacitor **S. Kumar**, S. Nandi, V. Mishra, A. Shukla and A. Misra	**Ms. Sumana Kumar**, Indian Institute of Science-Bangalore, **India**
16:45 - 17:00	Nanoparticles for High-Luminance Light-Emitting Diodes for Efficient Automotive Systems. **J.J.Santaella**, S.Rodríguez-Bolívar, L. Puga-Pedregosa, A. González-Rico, M. Marín-González and F.M.Gómez-Campos	**Dr. Juan J Santaella**, VALEO Lighting Systems, **Spain**
17:00 - 17:15	Complementary reduced Graphene Oxide-based inverter for ion sensing **R. Boukraa**, G. Mattana, N. Battaglini and B. Piro	**Mr. Rassen Boukraa**, ITODYS- Paris Cité University, **France**
17:15 - 17:30	Effect of 2D nanomaterials on MXene based engineered Aluminum plasmonic devices for bio-sensing in the near-infrared region **S. Shukla**, A. Verma, G. Karthiik, A. Sarkar and P. Arora	**Ms. Sambhavi Shukla**, Birla Institute of Technology and Science Pilani, **India**
17:30 - 17:45	An Unified Approach for Nanoplasmonics of Metal and Graphene-Based Nanostructures **T. Giovannini**, L. Bonatti and C. Cappelli	**Dr. Tommaso Giovannini**, Scuola Normale Superiore-Pisa, **Italy**
17:45 - 18:00	Two-dimensionnal substrate (MXene, graphene) supported nickel/iron-based catalysts for oxygen evolution reaction in alkaline medium L. Loupias, C. Morais, V. Mauchamp, S. Célérier and **A.Habrioux**	**Dr. Aurélien Habrioux**, University of Poitiers, **France**
18:00 - 18:15	Synthesis and Modeling of Supported Bimetallic Iron- and Copper Oxide nanoparticles and their Application in Fenton Reaction **B. Seynnaeve**, J. Lauwaert, P. Van Der Voort and A. Verberckmoes	**Mr. Bram Seynnaeve**, Ghent University, **Belgium**
18:15 - 18:30	Controlled loading of single atoms in oxygen vacancies as a co-catalyst on TiO2-x nanotube reduced by ultrasonication **M. Shahrezaei**, S. M. H. Hejazi, R. Zboril, A. Naldoni and S. Kment	**Mr. Mahdi Shahrezaei**, Palacký University, **Czech Rep**
18:30 - 18:45	Ternary phosphides (CuxCoyP) as efficient electrocataysts for HER and OER **D. Bandyopadhyay,** S. Ghosh and M. Bar-Sadan	**Ms. Dyuti Bandyopadhyay**, Ben-Gurion University of the Negev, **Israel**

June 16, 2022		
Nanotech / GAMS 2022 - Joint Session II.B - Nanocoatings/ Thin films and nanostructured surfaces		
Conference Room Moreau 1		
Session's Chairs: **Prof. Faruk Elaldi, University of Baskent, Turkey**		
08:30 - 09:00	A comparative study between blended polymers and copolymers as emitting films for single-layer white OLEDs D. Tselekidou, K. Papadopoulos, V. Kyriazopoulos, K.C. Andrikopoulos, A.K. Andreopoulou, J.K. Kallitsis and **M. Gioti**	**Prof. Maria Gioti**, Aristotle University of Thessaloniki, **Greece**
09:00 - 09:15	The influence of the nano-structured architecture type on the mechanical and tribological properties of TiN coatings **I. Borsan**, C; Gabor, M-A. Pop, F. Vaz and D. Munteanu	**Mrs. Ioana Borsan,** Transylvania University, Brasov, **Romania**
09:15 - 09:30	Dielectric Properties of Ca3Mn2O7 thin films prepared by Pulsed Laser Deposition **B. Silva**, J. Oliveira, T. Rebelo, P. Rocha-Rodrigues, N. Lekshmi, A. Lopes, J. Araújo, L. Francis and B. Almeida	**Ms. Bruna Silva**, University of Minho, **Portugal**
09:30 - 09:45	Reactivity at the interface between metals and Bi2Se3 topological insulator. **M. Fanetti**, K. Ferfolja, S. Gardonio and M. Valant	**Prof. Mattia Fanetti**, University of Nova Gorica, **Slovenia**
09:45 - 10:00	Preparation of nanostructured LiNbO3 containing nickel surface on silicon carrier by rotating disc electrode method **G. Dravecz** and L. Péter	**Dr. Gabriella Dravecz**, Wigner Research Centre for Physics, **Hungary**
10:00 - 10:15	Low Velocity Impact Behaviour of Composite Laminates Containing TiC and ZrC Nano-Particles in Resin System **F. Elaldi** and P. Alabay	**Prof. Faruk Elaldi,** University of Baskent, **Turkey**
10:15 - 10:30	Kinetically Controlled On-Surface Playground of Nanostructure Growth **A. Ahsan**, S. F. Mousavi, T. Nijs, S. Nowakowska, O. Popova, A. Wäckerlin, J. Björk, L.H. Gade, T. A. Junga	**Ms. Aisha Ahsan**, University of Basel, **Switzerland**
10:30 - 11:00	**Morning Coffee Break**	
Session's Chairs: **Prof. Faruk Elaldi, University of Baskent, Turkey** **Prof. Maria Gioti, Aristotle University of Thessaloniki, Greece**		
11:00 - 11:15	Core-shell nanofibers as coating re-inforcement **I. C. Vladu**, L. Balc and M. Sinnabell	**Mrs. Ioana Carmen Vladu**, Centre of Electrochemical Surface Technology (CEST), **Austria**
11:15 - 11:30	Intelligent coating systems on multimetallic composite structures for automotive production **N. Godja**, A. Schindel and L. Payrits	**Ms. Norica-Carmen Godja**, CEST, **Austria**
11:30 - 11:45	Correlation microstructure-heat treatments-mechanical properties of stainless steel 316L parts obtained by additive manufacturing **C. Ifounga**, M. Ben Azzouna and B. Lefez	**Mr. Claude Lajoie Ifounga**, Normandie University, **France**
11:45 - 12:00	An interaction study of epoxy varnishes with different metal oxides **G. Säckl**, J. Duchoslav, R. Pugstaller, C. Marchfelder, D. Stifter and G.M. Wallner	**Mr. Gary Säckl,** Johannes Kepler University Linz, **Austria**
12:00 - 12:15	Au nanoparticles coated Au/Ag mirror as SERS active substrate for trace chemical detection **V. Awasthi**, V. Bhardwaj, R. Goel and S. K. Dubey	**Mr. Vimarsh Awasthi,** Indian Institute of Technology Delhi, **India**

June 17, 2022

NanoMatEn - Session III. B
Nanotechnology for Energy/ Nanocatalysis (Part II)

Conference Room Derain 1+2

Session's Chairs:
Dr. Martynas Lelis, Lithuanian Energy Institute, Lithuania
Prof. Bassam Alameddine, Gulf University for Science and Technology, Kuwait

08:45 - 09:00	Rational synthesis and catalytic activity of bimetallic Ag/Pt nanoparticles **Y. Fan**, M. Waals, V. Noel, A. Girard, C. Salzemann and A. Courty	**Ms. Yinan Fan**, Sorbonne University, **France**
09:00 - 09:15	First evidence of lignin-pheomelanin nanostructured UVA driven synthesis of Pummerer's ketones by peroxidase mediated oxidative cou-pling of substituted phenols **S. Gabellone**, E. Capecchi, D. Piccinino and R. Saladino	**Dr. Sofia Gabellone**, University of Tuscia, **Italy**
09:15 - 09:30	Facing structural modifications in WO3 nanomaterials for improved light-responsive textiles **M. L. Pacheco**, T. V. Pinto, C. M. Sousa, A. Guedes, G. Blanco, J. M. Pintado, P. J. Coelho, C. Freire and C. Pereira	**Ms. Marlene Pacheco**, University of Porto, **Portugal**
09:30 - 09:45	Indium Phosphide Quantum Dots loaded on Mesoporous silica for Visible-Light Photo-Redox Catalysis **K. Bakkouche**, F. Ferrari, N. Katir, A. El Kadib, C. Nayral and F. Delpech	**Ms. Kaltoum Bakkouche**, INSA Toulouse, **France**
09:45 - 10:00	Design and Characterization of Cu and core-shell Cu@ZnO nanocatalysts **S. Hadaoui**, A. Naïtabdi and A. Courty	**Ms. Sonia Hadaoui**, Sorbonne University, **France**
10:00 - 10:30	**Morning Coffee Break**	

NanoMatEn - Session III.C
Nanotechnology for Environmental Application / Water treatment

Session's Chairs:
Prof. Prakash Mahanwar, Institute of Chemical Technology- Mumbai,India

10:30 – 11:00	Engineering of nanomaterials and membranes interfaces by Atomic Layer deposition: design, properties and applications **M. Bechelany**	**Dr. Mikhael Bechelany**, European Institute of Membranes of Montpellier, **France**
11:00 - 11:15	Fabrication of electrospun nanofibers based membranes and their use for CO2 capture **I. C. Vladu**, L. Balc, R. Wultsch, E. Hogger and C. Hansmann	**Mrs. Ioana Carmen Vladu**, Centre of Electrochemical Surface Technology (CEST), **Austria**
11:15 - 11:30	Design of nanocomposite based on halloysite for water treatment **M. Abid**, S. Sayegh, I. Latsunsky, E. Coy, G. Lesage, A. Ben Haj Amara and M. Bechlany	**Mr. Mahmoud Abid**, European Institute of Membranes of Montpellier, **France**
11:30 - 11:45	Development and characterization of porous calcium copper titanate membranes for water treatment **E. Makhoul**, F.Tanos, G. Lesage, M. Cretin, M. Boulos, D. Cornu and M. Bechelany	**Mrs. Elissa Makhoul**, European Institute of Membranes of Montpellier, **France**
11:45 - 12:00	Reiterative usage of bi-layered nanocrystaline carbon-doped TiO2 and Ni particles for the photocatalytic water treatment **M. Lelis**, M. Urbonavicius, S. Varnagiris, S. Tuckute and E. Demikyte	**Dr. Martynas Lelis**, Lithuanian Energy Institute, **Lithuania**
12:00 - 12:15	Conjugated microporous polymers using a copper-catalyzed [4 + 2] cyclobenzannulation reaction: promising materials for iodine and dye adsorption N. Baig, S. Shetty and **B. Alameddine**	**Prof. Bassam Alameddine**, Gulf University for Science and Technology, **Kuwait**

12:15 - 12:30	A comparison of unmodified and sawdust derived-cellulose nano-crystals (CNC) modified polyamide membrane using zeta potential and permeability **A. Adeniyi**, D. Gonzalez-Ortiz, C. Pochat-Bohatier and M. Onyango	**Dr. Amos Adeniyi**, Tshwane University of Technology, **South Africa**

June 17, 2022

Nanotech / Biotech - Session III. C
Nanotechnology for Drug and Gene Delivery

Conference Room Moreau 1

Session's Chairs:
Prof. Pilar Marco, IQAC-CSIC/CIBER-BBN, Spain
Dr. Isabella Tavernaro, BAM- Berlin, Germany

09:00 - 09:15	2D hybrid MnAl-fluorouracil nanotheranostic construct with controlled morpho-structural properties **B. Dragoi**, A. Ibanescu, R. Pomohaci, C.M. Uritu, D. Lutic and E. Carasevici	**Dr. Brindusa Dragoi**, Regional Institute of Oncology, **Romania**
09:15 - 09:30	Magnetic iron oxide nanoparticles for the delivery of thermal therapy for the treatment of primary aldosteronism **A. Sorushanova**, P. Donlon, O. Covarrubias, M. O'Halloran, P. Prakash, S. H. Boss-mann and M. C. Dennedy	**Dr. Anna Sorushanova**, National University of Ireland Galway, **Ireland**
09:30 - 09:45	pH-Responsive PAMAM Dendrimers Encapsulating Peganum harma-la Alkaloids and Tannic Acid with Improved Anticancer Activities as Compared to Doxorubicin **S. Ashraf Fahmy**, A. Sawy and H.M. El-Said Azzazy	**Dr. Sherif Ashraf Fahmy**, The American University in Cairo, **Egypt**
09:45 - 10:00	Multifunctional Polymer-Nanoparticle Composite for Wound Care Applications **R. Sanguramath**	**Dr. Rajashekharayya Sanguramath**, NSC-Nanosono Corp. Ltd, **Israel**
10:00 - 10:30	**Morning Coffee Break**	
10:30 - 10:45	Multifunctional nanogels containing SPIONs and miRNAs for wound healing and skin regeneration applications. The EuroNanoMed project TENTACLES A. Paolini, S.P. Bruno, A. Sobolevs, A. Plotniece, M.K. Chmielewski, L. Le Hégarat, K. Hogeveen, M. Sramkova, L. Balintova, A. Gabelova, A. Caporali, N. Cassinelli, B. Sanz, and A. Masotti	**Dr Andrea Masotti,** Children's Hospital Bambino Gesù, **Italy**
10:45 - 11:00	Synthesis and characterization of novel temperature-responsive bio-gels for microRNA delivery in wound healing applications. The TENTACLES project **A. Paolini**, S.P. Bruno, A. Sobolevs, A. Plotniece, M.K. Chmielewski, L. Le Hégarat, K. Hogeveen, M. Sramkova, L. Balintova, A. Gabelova, A. Caporali, N. Cassinelli, B. Sanz and A. Masotti	**Dr. Alessandro Paolini**, Children's Hospital Bambino Gesù, **Italy**
11:00 - 11:15	Nanostructured semiconductor CuO(1−x)ZnOx nanocomposite with a broad spectrum antibacterial activity and its application in medical devices and acrylic paints **A. Franco**	**Dr. Ariel Franco**, NSC-Nanosono Corporation Ltd, **Israel**
11:15 - 11:30	Assessment of occupational exposure to nanoparticles during the de-velopment of enhanced materials for metal additive manufacturing **C. F. Martins**, J. Laranjeira, C. Matos, A. R. Alberto, J.J. Rosero-Romo, S. Martin-Iglesias, U. Silvan and D. Salazarb	**Dr. Carla Martins**, ISQ Institue, **Portugal**
11:30 - 11:45	Wound dressing based on cellulose sponges incorporated with curcumin-β-cyclodextrin inclusion complex and chitosan **K. Kiti** and O. Suwantong	**Mr. Kitipong Kiti**, Mae Fah Luang University, **Thailand**
11:45 - 12:00	pH-Responsive Dissociable Nanoscale Coordination Polymer for Diagnosis and Treatment of Atherosclerosis **Y. Lin**, S. Yen Chong, J. Liu, C. Huang, B. Liu, J. C. Yong Kah and J-W. Wang	**Mr. Yuanzhe Lin**, National University of Singapore, **Singapore**

Posters Session

Posters are to be displayed through the event platform solution (Whova App).
Discussions are to be done through the system chat features available to the attendees.

N.	Title	Author / Affiliation / Country
1.	Synthesis and Characterization of Phenanthroimidazole Derivatives with Amphiphilic Chains **R. Butkute**, D. Volyniuk and J.V. Grazulevicius	**Dr. Rita Butkutė**, Kaunas University of Technology, **Lithuania**
2.	Production of self-assembled Ag nanoparticles in SiC matrix **T. Car**, S. Isaković, I. Periša and S. Bernstorff	**Dr. Tihomir Car**, Ruđer Bošković Institute, **Croatia**
3.	Application of Cationic CNC and Nafion Membrane in the Electrolysis of Salt Solution G. Joong Kim and **Y. Ryeong Oh**	**Ms. Ye Ryeong Oh**, Inha University, **Rep. of Korea**
4.	Numerical studies of injection moulds for the production of bonded magnets **J. Silva**, D. Campanhã, J. Fonseca, J. Camarinha, D. Dias, P. Costa and M. Silva	**Mr. José Silva,** Centre for Nanotechnology and Smart Materials, **Portugal**
5.	Strain-induced direct to indirect bandgap crossover in monolayer WSe2 **H-Y. Hwang**, I-H. Kim, R.J. Taylor, K S. Kyhm	**Dr. Hyeong-Yong Hwang**, University of Oxford, **UK**
6.	Low-temperature amorphous silicon deposition by DC sputtering M. Sun, **S. Valdueza-Felip** and F. B. Naranjo	**Dr. Sirona Valdueza Felip**, University of Alcala, **Spain**
7.	Functionalization of Fiber Bragg Grating Using Different Coating Methods **V. Kumar** and S. Asokana	**Mr. Vajresh Kumar**, Indian Institute of Science- Bangalore, **India**
8.	Effect of Ag Doping on Threshold Switching Characteristics of Amorphous Ga2Te3 Film **J. Kim**, M. Kang, W. Kim and H. Sohn	**Mr. Jaeyeon Kim**, Yonsei University-Seoul, **Rep. of Korea**
9.	Exploring Bismuth Plasmonics In The Visible Spectrum **D. E. Martínez-Lara**, R. González-Campuzano and D. Mendoza	**Mr. David Eduardo Martínez Lara**, The National Autonomous University of Mexico, **Mexico**
10.	Applicability of low-cost FPGA boards in custom built Scanning Probe Microscopy electronics **M. Valtr** and P. Klapetek	**Dr. Miroslav Valtr**, Czech Metrology Institute, **Czech Rep**
11.	Investigation of chemical reduction graphene oxide for supercapacitor application. Systematic research **T. Chudziak**, W. Czepa, D. Pakulski, A. Musiał, C. Valentini, M.Bielejewski, P. Samorì and·A. Ciesielski	**Mr. Tomasz Chudziak**, Adam Mickiewicz University, **Poland**
12.	CNO-induced organization of well-defined star block polymers to ob-tain mesoporous carbon materials and their application in electrochemistry **G. Siemiaszko**, A. Hryniewicka, J. Breczko, M. E. Plonska-Brzezinska	**Dr. Gabriela Siemiaszko**, Medical University of Bialystok, **Poland**
13.	Synthesis of highly ordered carbonaceous materials with controlled formation of specific pore diameters and their application in electro-chemistry and electrocatalysis **J. Breczko**, G. Siemiaszko, A. Hryniewicka and M. E. Plonska-Brzezinska	**Dr. Joanna Breczko**, Medical University of Bialystok, **Poland**
14.	Combined effect of multiple atomic interactions and structural catalysis on the H release from MgH2 in Mg-Ni-rGO system **S. Panda**, V.V. S. A Marla and S. S. V. Tatiparti	**Mr. Srikanta Panda**, Indian Institute of Technology Bombay, **India**
15.	Structural and dielectric properties of CoFe2O4\BaTiO3 Bilayers deposited over highly doped Si(001) substrates **J. Oliveira**, B. Silva, J.A. Mendes and B.G. Almeida	**Mr. João Oliveira**, University of Minho, **Portugal**
16.	Strong grain boundary non-radiative recombination peak around the angle (35°) of EBSD disorientation in CdSeTe thin-film Photovoltaics **T. Altamimi** and B. Mendis	**Ms. Taghreed Altamimi**, Durham University, **UK**
17.	Nanostructured metal (Cr, Zr, Co) nitride thin film electrodes sputtered grown for excellent energy storage devices **R. Adalati**, M. Sharma, A. Kumar, S. Sharma and R. Chandra	**Mr. Ravikant Adalati**, Indian Institute of Technology Roorkee, **India**

18.	Ink-Jet Printed TiO2 Thin Layers with Embedded Au Nanoparticles as Functional Layers for Perovskite Solar Cells **S. Rubtsov**, A. Musin, M. Zinigrad and V. Danchuk	**Mrs. Sofia Rubtsov,** Ariel University, Israel
19.	Development of a measurement method of voids in printed patterns to assess printability **C. Hwan Kim**	**Prof. Chung Hwan Kim**, Chungnam National University, **Rep. of Korea**
20.	Copper Silicide/SnSb Core-Shell Nanowires as a High-Capacity Material for Sodium-Ion Battery Anodes S. O'Sullivan, K.M. Ryan, H. Geaney and **T. Kennedy**	**Dr. Tadhg Kennedy**, University of Limerick, **Ireland**
21.	Enhancing long-term photostability of BiVO4/CdS photoanodes **H. Kmentova**, R. Yalavarthi, A. Naldoni and S. Kment	**Dr. Hana Kmentova**, Palacky University- Olomouc, **Czech Rep.**
22.	Effect of experimentally verified nanofluid electrolytes to improve the electrochemical properties of flow batteries **J. Kim** and H. Park	**Dr. Jungmyung Kim**, Changwon National University, **Rep. of Korea**
23.	Ultrafast laser-based fabrication of Efficient Anti-reflective Silicon Nitride nano/microstructures for Optoelectronics applications **P. Malik**, S. Ghosh, G.V. Prakash and P. Srivasatava	**Ms. Pariksha Malik**, Institute of Technology Delhi, **India**
24.	In-silico design of graphene plasmonic hot-spots **L. Bonatti**, L. Nicoli, T. Giovannini and C. Cappelli	**Mr. Luca Bonatti**, Scuola Normale Superiore- Pisa, **Italy**
25.	CuInS/ZnS Core-Shell Quantum Dots A Green Alternative to Cd and Pb Core-Shell Quantum Dots **K.J. Knebel**, J.R. Montes-Bojorquez and A. Ayon	**Mr. Kevin Knebel**, The University of Texas San Antonio, **USA**
26.	Advancements in white electroluminescent carbon dot- based light emitting diodes **O.Ligor**, D. Bogosel, E.M. Pavelescu, A. Istrate, F. Nastase, I. Mihalache, E. Vasile, A. Terec and L.M.Veca	**Dr Octavian Ligor**, National Institute for Microtechnology- Bucharest, **Romania**
27.	Phenothiazinyl-substituted Bis(trifluoromethyl)biphenyl Compound for Efficient Oxygen Sensing **R. Keruckiene**, N. Kusas, V. E. Matulis and J. V. Grazulevicius	**Dr. Rasa Keruckienė**, Kaunas University of Technology, **Lithuania**
28.	Advanced materials based on azulene-phenyloxazolone **A.G. Brotea**, C. Musina (Borsaru), O.T. Matica, M. Cristea, E.-M. Ungureanu and A. Stefaniu	**Ms. Alina-Giorgiana Brotea**, University "Politehnica" of Bucharest, **Romania**
29.	Synthesis and repetitive application of nanocrystalline ZnO based floating photocatalyst for the detoxification of water from bacteria and viruses mixtures **M. Lelis**, S. Tuckute, E. Demikyte, D. Vasiliauske, M. Urbonavicius, S. Varnagiris and S. Sakalauskaite	**Dr. Martynas Lelis**, Lithuanian Energy Institute, **Lithuania**
30.	Investigation of bi-layered ZnO-Ni photocatalyst powder produced by reactive magnetron sputtering technique **M. Lelis**, S. Tuckute, E. Demikyte, D. Galalyte, R. Daugelavicius and S. Sakalauskaite	**Dr. Martynas Lelis**, Lithuanian Energy Institute, **Lithuania**
31.	Reduced graphene oxide/gold nanoparticles nanocatalyst: Applications for Suzuki reactions in water and oxidative esterifications **R. Pocklanova**, M.B. Gawande and L. Kvítek	**Mrs. Radka Pocklanova,** Palacky University- Olomouc, **Czech Rep.**
32.	Immobilized functionalized silver nanoparticles to detect Cadmium in water. **D.Mondal** and S.Asokan	**Mr. Debojyoti Mondal**, Indian Institute of Science- Bangalore, **India**
33.	The Possibility of Reactive Printing on Inherent Flame Retardant Fabrics **V. Lovreškov**, M. I. Glogar, T. Kaurin, T. Pušić and N. Kerman	**Ms. Veronika Lovreškov**, University of Zagreb Faculty of Textile Technology, **Croatia**
34.	Flame retardant and surface properties of designed aramid fabrics T. Kaurin, T. Pušić, M. I. Glogar, V. Lovreškov, Z. Kovačević and N. Kerman	**Ms. Tea Kaurin**, University of Zagreb Faculty of Textile Technology, **Croatia**
35.	Surface properties of polyester fabrics **A. Šaravanja**, T. Dekanić, T. Pušić, T. Kaurin, K. Grgić and M. Čurlin	**Ms. Ana Saravanja**, University of Zagreb Faculty of Textile Technology, **Croatia**
36.	Benefits of low-temperature aging of superelastic NiTi alloy **O. Tyc** and P. Šittner	**Mr. Ondrej Tyc**, Institute of Physics of the Czech Academy of Sciences, **Czech Rep.**

37.	Surface degradation study of historical crown glasses from 15th – 17th century **A. Nowicka**, E. Greiner-Wrona, B. Hruška, M. Chromčíková and M. Liška	**Dr. Aleksandra Nowicka**, Alexander Dubček University, **Slovakia**
38.	Thermomechanical properties of silicate and phosphate glasses **M. Chromčíková**, B. Hruška, A. Novicka, B. Pecúšová and M. Liška	**Mrs. Mária Chromčíková**, Alexander Dubček University, **Slovakia**
39.	The surface layer study of binary glasses. **B. Hruška**, T. Gavenda, A. Nowicka, M. Chromčíková and M. Liška	**Dr. Branislav Hruška**, Alexander Dubček University, **Slovakia**
40.	Zn-rich coatings dried with infrared (IR) radiation I. Stojanović, **I. Cindrić**, L. Turkalj, I. Juraga, M. Kurtela, V. Šimunović, V.Alar and H. Franjić	**Mr. Ivan Cindrić**, University of Zagreb, **Croatia**
41.	Bioactive spray based on green synthesis silver nanoparticles **A. Ounkaew** and P. Kasemsiri	**Ms. Artjima Ounkaew**, Khon Kaen University, **Thailand**
42.	Aspergillus for nanoparticle: Possibilities and challenges of biomediated nanoparticle synthesis of silver nanoparticles **J. Walter**, I. Aubel and M. Bertau	**Mr. Jan Walter**, University of Mining and Technology Freiberg, **Germany**
43.	Peptide Targeted Gold Nanoplatform Carrying miR-145 Induce Anti-tumoral Effects in Ovarian Cancer Cells E. Salas-Huenuleo, A. Hernández, L. Lobos-González, I. Polakovicova, F. Morales-Zavala, F. Celis, **P. Valenzuela-Bustamante,** C. Romero and M. J. Kogan	**Ms. Paula Valenzuela Bustamante**, Advanced Integrated Technologies, **Chile**
44.	Brain Drug Delivery of Riluzole by means of Lactoferrin Functionalized Nanostructured Lipid Carriers **M. I. Teixeira**, C. M. Lopes, M. H. Amaral and P. C. Costa	**Ms. Maria Inês Teixeira**, University of Porto, **Portugal**
45.	Innovative biogels delivering miRNAs into skin models. Wound healing applications within the EuroNanoMed project TENTACLES **S.P. Bruno**, A. Paolini, A. Sobolevs, A. Plotniece, M. K. Chmielewski, L. Le Hégarat, K. Hogeveen, M. Sramkova, L. Balintova, A. Gabelova, A. Caporali, N. Cassinelli, B. Sanz and A. Masotti	**Ms. Stefania Paola Bruno,** Children's Hospital Bambino Gesù, **Italy**
46.	Design Optimization of Memantine Loaded Micro/Nanomotor for Alzheimer's Disease G. Tezel, E. Öztürk, S. Seda Timur, R. N. Gürsoy, K.Ulubayram, L. Öner, **H. Eroğlu** and F. Kuralay	**Prof. Hakan Eroglu**, Hacettepe University, **Turkey**
47.	Protein aggregation mechanisms: human H-ferritin self-assembly for constructions of new nanomaterials **R. Lucignano** and D. Picone	**Ms. Rosanna Lucignano**, University of Naples Federico II, **Italy**
48.	Targeting Iron Metabolism in Cancer to Induce Ferroptosis: A Type of Programmed Cell Death **R. Beadman**, M. Bilbao-Asensio, J. Mareque-Rivas, I.M. Sheldon and J. Cronin	**Ms. Rhiannon Beadman**, Swansea University, **UK**
49.	Antibacterial chitosan-graphene nanocomposites **N. Wrońska**, A. El Kadib and K. Lisowska	**Dr. Natalia Wrońska**, University of Lodz, **Poland**
50.	Synthesis of PLGA, PCL and its Nano-Fabrication for the Tissue Engineering Application by using Electrospinning and Melt Pining Technique **S.H Bansode** and P. A Mahanwar	**Ms. Savita H Bansode**, Institute of Chemical Technology- Mumbai, **India**
51.	Recycling of used face mask to white light emitting carbon dots **M. Perikala** and A. Bhardwaj	**Ms. Manasa Perikala**, Indian Institute of Science, Bangalore, **India**
52.	Rapid, accurate detection of COVID-19 utilizing novel isothermal nucleic acid amplification **Y. Ju**, J. Kim, Y. Park, C. Y. Lee, K. Kim, K. H. Hong and H. G. Park	**Mr. Yong Ju**, Korea Advanced Institute of Science and Technology, **R. of Korea**
53.	Titanium Coating on Laser Roughened PEEK for Spinal Implant H-K. Tsou, **P-Y. Hsieh** and J-L. He	**Dr. Ping-Yen Hsieh**, Feng Chia University, **Taiwan**
54.	Lipase-catalyzed acylation of bio-oil enriched with levoglucosan: antibacterial and biosurfactant studies	**Mr. Marcelo A. do Nascimento**, Centrale Lille Institute, **France**

	M.A. do Nascimento, R. Froidevaux, R. Wojcieszak, R.O. M. A de Souza and I.I. Junior	
55.	Heterotrophic growth of the red microalga Galdieria Sulphuraria **M. van der Hoek**, I. Kristijarti, A. van Wijk, and M.J.E.C. van der Maarel	**Ms. Mariska van der Hoek**, University of Groningen, **The Netherlands**
56.	Flexible Alternatives To Process Intensification For mAb Purification S; Bola, W.H. Rushton, **J-F. Depoisier** and J.C. Greenwood	**Mr. Jean Francois Depoisier**, Bio-Rad Laboratories, **France**
57.	Bacteria attacking plastic waste E. Noel, S. Amghar, S. Douay, S. Taktek and **H. Horchani**	**Prof. Habib Horchani**, Cégep de Rivière-Du-Loup, Quebec, **Canada**
58.	High level expression and characterization of extracellular lipase Lip7 from *Yarrowia lipolytica* A. Biegalska, Z. Lazar and **T. Janek**	**Dr. Tomasz Janek**, Wrocław University of Environmental and Life Sciences, **Poland**
59.	Synthesis of Gold Nanoparticles and Field-Resolved Metrology for the Investigation of Localized Surface Plasmons **D. Schauer**, D. Zimin, J. Bredehoeft and H. Jakob Wörner	**Mr. David Schauer**, ETH Zurich, **Switzerland**

Nanotech / GAMS
Joint Plenary session

Using 2D materials in a 3-dimensional world: from nanochemistry to technology applications

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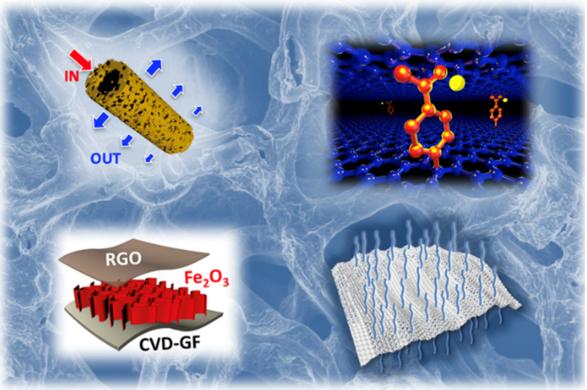
Abstract:

In this talk, I will give an overview on how our group uses 2-dimensional nanosheets of graphene and related materials as a versatile chemical platform to develop novel 2-dimensional composites, and how such composites can be used in disruptive applications in the fields of automotive, aeronautics, water and gas purification and electronics.

The 2-dimensional shape of graphene can be used to create unique 2D composites formed by stacked multilayers of graphene alternated to other small molecules, polymers, nanoparticles, metal oxides, enzymes etc., materials which would be impossible to make with conventional 3D materials or 1D polymers. Molecules and ions can penetrate and diffuse in between these 2D nanosheets, allowing applications that span from energy storage, to water purification, to gas separation. I will describe how, using novel techniques based on electrochemistry, solution processing and surface chemistry, it is possible to create novel composite architectures spanning from the nano- to the macro-scale.

Using this approach, there is practically no limit to the number of possible 2D structures inspired to graphene which shall be created.



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LEGO chemistry for graphene-based nanoarchitectures: from 0D quantum dots to 2D lateral heterostructures

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Abstract:

Bottom-up nanoarchitectonics has demonstrated the capability to control structural parameters of nanomaterials with atomic precision. The surface-assisted synthesis of graphene-based one-dimensional nanostructures à la carte distinctly illustrates the power of this concept. However, despite impressive advances in the synthesis of 1D homostructures, advancing in structural complexity faces major challenges. The functionalization of edges in nanoribbons, an effective strategy to tailor their electronic properties and chemical interactions, is a clear example. The concept of inserting the desired functional groups or dopants in the molecular precursor often fails due to their lack of stability during the reaction path. The fabrication of heterostructures is a second example, where the challenge lies on the control of the size and distribution of their components. A third one is extending the on-surface strategy to two-dimensional structures, where examples of long-range ordered nanoarchitectures are very limited.

I will present different strategies that we developed to overcome each one of this challenges. Regarding edge functionalization, we recently synthesized pyrimidine functionalized ovalene quantum dots, and amino [1] and fluorine [2] functionalized graphene nanoribbons, demonstrating that this strategy is effective for tailoring the electronic band structure. We have also developed a method to synthesize a 2D nanoporous graphene, where the long-range order is achieved by the sequential growth of 1D building blocks and their posterior coupling [3]. Most recently, we have synthesized a Nitrogen doped nanoporous graphene structure that electronically behaves as a 2D superlattice heterostructure [4]. The particular electronic properties of the heterocomponents and the interface structure results in atomically sharp band discontinuities that host subnanometer quantum dipoles, altogether enabling the realization of 1 nm scale superlattice heterojunctions.

Keywords: on-surface synthesis, graphene nanostructures, scanning tunneling microscopy.

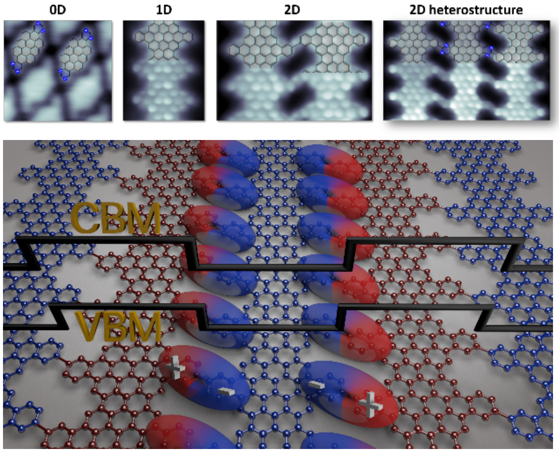

Figure 1: (Top) From 0D to 2D graphene nanoarchitectures. (Bottom) Schematics of a graphene-based lateral heterostructure with nanometer scale components and atomically sharp structural and electronic junctions.

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0D + 1D = 2D: Heterogeneous Electrodes by Electrospinning

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Abstract:
Major advances in catalytic coatings and membranes and in electrocatalytic electrodes are resulting from our ability to design and fabricate heterostructured multiphase materials of high specific surface area [1,2]. Such advances are needed to realize the full potential of 2D materials, and these advances require symmetry-breaking during fabrication. We have begun to develop and demonstrate how nonwoven mats made by electrospinning can advance beyond the inherent 1D fibers intrinsic to electrospinning. We have disclosed [3] how to coat 2D materials, for example graphene nanosheets, in randomly oriented networks with nanofiber network connectivity, so that the 2D anisotropy inherent to such nanosheets is retained in the resulting coatings. This anisotropy result emanated from a hydrodynamic linear instability effect (driven by spontaneously decreasing of surface free energy to minimize the surface area to volume ratio) manifested intermittently with the preferred electrospinning. Here we further capitalize on operating close to such a hydrodynamic instability boundary between electrospraying and electrospinning. We discuss electrospinning of a multiphase aqueous suspension composed of 0D nanolatexes (NLs), 1D MWCNTs (multiwall carbon nanotubes), and an aqueous solution of PVA (polyvinyl alcohol). Rather than obtaining a typically fibrous web of predominantly 1D anisotropy, we obtain a randomly oriented network of 2D nanomembranes supported by MWCNT and bound by mixtures of NL and PVA. An example volume element of such a coating is illustrated in Figure 1. The 2D components are μ-films that are formed by PVA and NL that remain after drying and are remnants of menisci supported by mini-networks of MWCNTs. The internal structure of these μ-films has not been fully resolved, but morphological aspects are resolved at higher magnification. These images suggest a redistribution of NLs during multiphase suspension formation, electrospinning, and drying that transfers NLs from MWCNT surfaces to the product-2D μ-film surfaces supported between MWCNTs within NL-PVA μ-films. Approaches to structural tuning, improving electrochemical properties, and directions for future applications are discussed and include film densification to modify specific surface area, carrier and NL modification to modulate ionic and electrical conductivities, and nanophase doping to create further heterostructures that facilitate tandem support of additional catalytic sites for tandemly consecutive reaction catalysis. These observations provide a basis for increasing dimensionality and designing 2D networks based on coupling a hydrodynamic instability with colloidal network re-equilibration rather than by diffusion-limited aggregation.

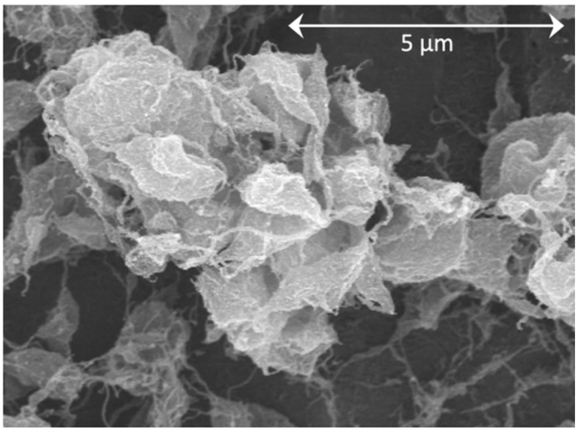

Figure 1: SEM of heterostructured 0D nanolatex + 1D MWCNT coating using PVA carrier fluid.

Keywords: nanolatex, multiwall carbon nanotube, MWCNT, graphene, heterostructres

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Synthesis of (multi-)Metal core-shell and alloyed nanoparticles by atmospheric pressure plasma filament-surface interaction

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Abstract: Local and transient heating of solid targets by lasers and sparks (1-100 mJ per pulse) induces fluencies above the threshold one for vaporization of any solid material. Both are thus used at industrial scale for nanomaterial processing using nanoparticles (NP) production by nucleation of vapors from any material.

Taking advantage of the large range of energy that can be induced in non-thermal plasma filaments, the presentation highligths the interest of different atmospheric pressure plasmas for the synthesis of Metal NP by nucleation in Nitrogen. Starting with mono-Metal NP produced by DC streamers and sparks versus the energy per filament (0.1-100mJ)[1], the interest of Dielectric Barrier Discharge with lower energy per filament (0.1-100μJ) is highlighted for the synthesis of ***single digit nanometer sized primary nucleated Metal Nanoparticles***.

The mechanisms of particle formation are briefly depicted with respect to both types of particles systematically formed by transient atmospheric pressure plasma filaments (from a few ns to a fraction of ms), interacting with metal electrodes: (i) few solidified submicron sized droplets are directly ejected from molten craters from a tenth to few μm. (ii) Surface vaporization of any materials (oxides, metals and polymers) also occurs with respect to single digit nanometer sized primary nucleated particles and subsequent 10 to 100nm agglomerates grown by agglomeration.

Mechanisms of NP production and evolution are then addressed with respect to size distributions, composition from EDX and cristalinity from SAED characterization of NP produced by less energetic filaments (referred as microdischarges) in Dielectric Barrier Discharges on Au, Cu Ag[2]. Then, amorphous and crystalline pure primary NPs are produced by physical nucleation in expanding vapors jets. Finally, NPs with single digit diameters (< 5nm) are formed by agglomeration of primary nuclei in each vapor plume and during the transit between filaments. The first local agglomeration can be limited by lowering the initial vapor flux at reduced energy per filament, while the second growth step depends on transit times in the discharge gap. DBD is a simple atmospheric pressure, chemical-free plasma process to produce NPs with tunable size and the same composition than the electrode.

The presentation then foccusses on multi-Metal NP synthesis with sparks on alloys.
Despite very different evaporation temperatures of both metals in $CuZn_x$ alloys, plasma-alloys interaction leads to core-shell NPs. Indeed, Cu@Zn NP are formed, then oxidized during storage in air before analysis. The core is made of the more condensable of both metals, i.e. Cu with the lower saturation vapour pressure (P_{sat}) than Zn, which condense later on the Cu core.

With alloys of metals with close evaporation temperature and saturation vapour pressure, biM-alloyed NP can be procesed with the same stoichiometry than for instance the Co-Ni alloys submitted to sparks. These amorphous NP can be cristalised by post-plasma sintering of suspended NPs in an tubular furnace at 1100°C for 30''.

Keywords: plasma filaments (streamer, spark, microdischarge), surface heating, crater melting, submicron solidified droplets, vaporization, nucleation, NP agglomeration, metal, alloys, core-shell.

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Nanotech / GAMS Joint Session I.A: Nanomaterials Fabrication / Synthesis / properties

Addressing magnetic and topological properties of graphene nanoribbons

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Abstract:

Graphene nanoribbons (GNRs) are quasi-1D strips of graphene, and constitute a novel platform for carbon-based nanoelectronics. The atomically precise bottom-up shaping of GNRs is now possible by on-surface synthesis methods, which unite the sturdiness of covalently bonded networks with the easy tunability of molecular materials.[1] This unprecedented level of control of the overall lattice and chemical structure has given rise to the exploration of novel features in GNRs, such as magnetic states and topological phases.

In this talk, I will review some of our recent works on GNRs, performed in close collaboration with our experimental colleagues. Using Density Functional Theory (DFT) and model calculations, we have investigated the electronic, magnetic and topological properties of different types of GNRs. Our theoretical results are supported by Scanning Tunneling Microscopy (STM) experiments.

In semiconducting armchair GNRs, we explore the emergence of magnetism upon substitutional doping with boron atoms.[2] Furthemore, it is possible to tune the boron-induced magnetic states by slight modification of the GNR's morphology. For semi-metallic chiral GNRs, we demonstrate the occurrence of a topological phase transition upon varying their width.[3] Our findings emphasize the potential of GNRs for quantum electronic and spintronic applications.

Keywords: graphene nanoribbons, density functional theory (DFT), scanning tunneling microscopy (STM), magnetism, topology.

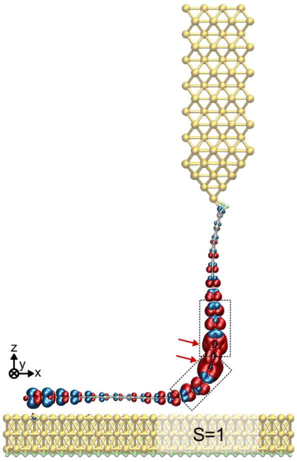

Figure 1: DFT optimized structure of an armchair GNR doped with a pair of boron atoms, and contacted by a STM tip. Magnetization isosurfaces are shown over the atomic structure.

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One-step Elaboration of Janus Polymeric Nanoparticles

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Abstract:

Particles having biphasic geometry of various chemistries, composition and/or functionalities are called "Janus particles",[1] inspired by the eponym two-faced Roman god. This anisotropic nature gives rise to unique properties, which made these particles very useful in a wide range of applications, such as biosensing,[2] theranostics[3] or smart textiles[4]. This type of particles is generally obtained after several steps (the particles' elaboration and the surface functionalization) sometimes needing hard chemical solvents and leading to the elaboration of emulsions with large and multi-modal sizes distributions.

In this study, we prepared polymeric Janus nanoparticles (JNPs) by a one-step method from a mixture of two different polymers and to compare several emulsification-evaporation processes (sonication, shear mixing and elongational-flow micromixing). Process and physical-chemistry parameters highly influenced the JNPs size and morphology.

The possibility to obtain monomodal JNPs with a diameter lower than 200 nm, with a hydrophobic domain (poly(lactic-co-glycolic acid)) and a hydrophilic charged domain (based on poly(styrene sulfonate)) was demonstrated with the elongational-flow micromixer.

Keywords: Janus nanoparticles, biocompatible polymers, emulsification, elongational-flow micromixer, interfacial chemistry, chemical engineering

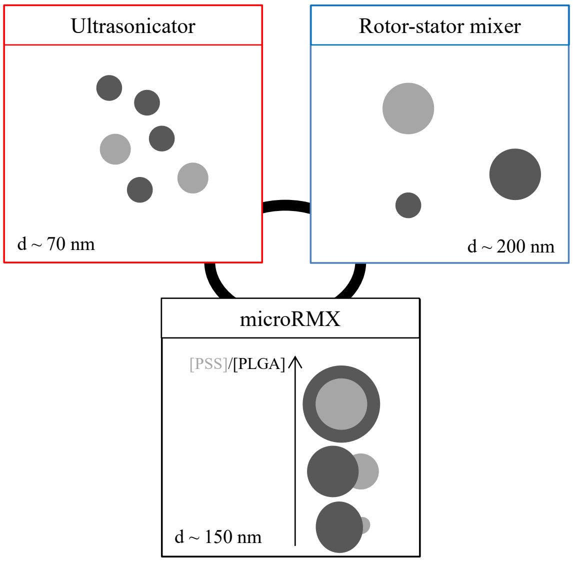

Figure 1: The different morphologies obtained with the three devices used in the presented study.

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Calix[4]arene-Tetradiazonium Salts: a Powerful and Versatile Tool for Nanomaterials Functionalization.

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Abstract:

Nanomaterials and especially plasmonic nanoparticles are more and more studied in the biomedical field. This increasing interest lies in their remarkable chemical and optical properties resulting from their nanosize. In particular, gold nanoparticles (AuNPs) exhibit a localized surface plasmon resonance (LSPR) band in the visible region, which strongly depends on the dielectric properties of their local environment. In addition, several chemistries are known that allow their functionalization with a large variety of biomolecules (peptides, proteins, DNA, polymers, ...). These features gave rise to numerous developments as nanocarriers for in vivo drug delivery, hotspots for phototherapy, contrast agents for imaging systems, or colorimetric reporters for *IVD*. For all these applications, AuNPs must be engineered to (i) possess sufficient chemical and colloidal stabilities and (ii) express specificity for target molecules or tissues. This grafting is usually achived via thiol chemistry, as it is a very convenient grafting strategy based on the formation of Au−S bonds. However, thiol chemistry possesses two severe drawbacks limiting their use for in vivo applications: (i) a limited chemical robustness of the organic layer due to the lability of the Au−S bond and (ii) the difficulty to control the grafting density of different thiolated molecules on the AuNP surface.[1]

We recently developed a nanoparticle functionalization strategy taking advantage of calix[4]arene-tetradiazonium salts.[2] We have shown that thin layers of these molecular platforms can be strongly and irreversibly grafted to the NP surface via the reduction of their diazonium groups that leads to the formation of multiple covalent bonds. Furthermore, as calix[4]arene-tetradiazonium salts differently substituted on the phenol positions possess a similar reactivity for gold surfaces, it was shown that the composition of mixed layers of calix[4]arenes could be controlled on AuNPs[3], allowing the control of the grafting density of biomolecules on their surface.[4] This strategy could further be extended to synthesize silver and alloyed gold-silver nanoparticles,[5] displaying high colloidal and chemical stabilities, despite the thinness of the organic layer, and a controlled bioconjugation capacity. These silver nanoparticles could be functionalized with peptide aptamers and used to detect a cancer biomarker, the protein Mdm2, using a dual-trapping aggregation based assay in biologically relevant conditions, paving the way for the use in colorimetric nanosensors.[6]

Keywords: nanoparticles coating, calixarene-diazonium salts, gold nanoparticles, silver nanoparticles, colorimetric sensors.

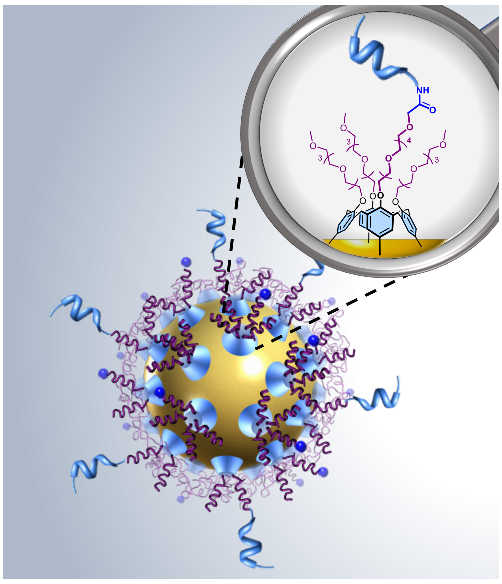

Figure 1: Schematic representation of the nanoparticle functionalization strategy based on calixarene salts .

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Mass producing of TEMPO oxidized nanofibers from thermomecanical pulp for various applications: global approach needed

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Abstract:

Uses of wood derivatives in various applications is a good pathway to reach stringent environmental goals and, furthermore, promote fossil product replacement. Many research groups have developed new applications with nanocelluloses produced from chemical pulp, composed almost exclusively of cellulose. Especially in North America, thermomechanical pulp (TMP) is another important pulp market. From the various paper market modifications, namely hard newsprint volume reduction, mills capacity is now available for other usages. With a successful chemical modification by a 4-acetamido-TEMPO oxidation, we have being producing low or highly charged nanofibers from TMP (Figure 1). Having developed a few potential applications, namely paper reinforcement and increased filler retention at low oxidation level or flexible and conductive composites at high oxidation level [1,2], we have researched and developed a semi-industrial nanofibers production process using a conventional TMP production line (Figure 2) [3].

While the oxidation could not be directly implanted in the usual TMP process and would require process modifications, we found that a TMP refiner can be used as a very efficient disperser to produce significant quantities of nanofibers. However, the TEMPO solution must be reused in order to achieve economic profitability. From our present lab scale research, TEMPO solution recycling cannot be done solely on one of the presented applications. Recycling of the TEMPO solution was possible a maximum of 2 times at high carboxylic groups content (film and composite applications) and up to 8 more times at low oxidation level. From our result, it is obvious that if a TEMPO process is indeed used on an industrial scale, the mills would have to produce an array of products and not only a single one to achieve profitability.

Keywords: Thermomechanical pulp, nanofiber, TEMPO oxidation, composite, paper, semi-industrial production, recycling

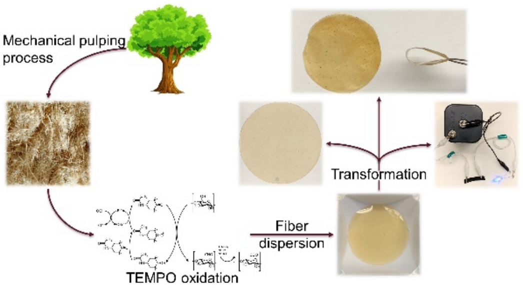

Figure 1: General approach of the films/composites research.

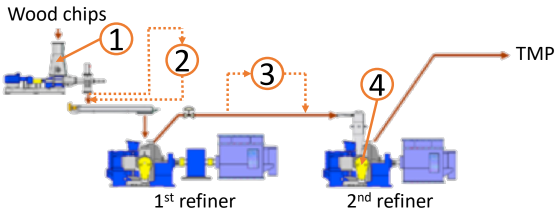

Figure 2: TEMPO solution injection point in our pilot TMP process.

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Synthesis, characterization and industrial application of a nanofluid based on copper nanoparticles with long-lasting antimicrobial effect

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Abstract: In recent years, interest in the industrial uses of metallic nanoparticles has increased due to their special chemical and physical properties and their potential applications in diverse fields including electrochemistry, medicine, catalysis, and electronics. Among the most used metals to synthesize nanoparticles are gold and silver, while copper has positioned itself as a highly valued material due to its characteristics such as high conductivity, low cost and high antimicrobial effectivenes[1,2]. In addition, due to the growing demand for disinfectant products worldwide, the search for active ingredients with antimicrobial properties has increased. In the case of Cu^{+2}, metallic copper nanoparticles structured in a stabilizing matrix can be oxidized by air and the formed cations diffuse from the matrix and inhibit microorganism[3]. The objective of our work was to develop a broad spectrum antimicrobial nanofluid based on copper nanoparticles at industrial level. The synthesis process consisted of a chemical reduction with organic acids, in the presence of a cationic surfactant as a capping agent, with controlled conditions of temperature, agitation and concentrations. This process was scaled-up to produce a stable nanofluid on an industrial scale. The copper nanoparticles presented narrow size distribution with an average of 2.5 nm determined by DLS and TEM, a diffraction pattern correlated with metallic state and a purity greater than 99.9%. The antimicrobial efficacy has been evaluated on different porous and non-porous surfaces, both in various national and international studies. Other studies have shown the residual effect of copper nanoparticles, which have been effective in reducing bacterial growth by 99.9999% up to 7 days after single application (Figure 1). These results have given rise to a long-lasting antimicrobial nanotechnology, which is in the process of being patented and has been consolidated in a disinfectant product called DECUTEC. Finally, it should be noted that various products based on our nanotechnology have been developed and registered, demonstrating the industrial applicability of copper nanoparticles.

Keywords: copper nanoparticle, antimicrobial, scale-up, industrial application

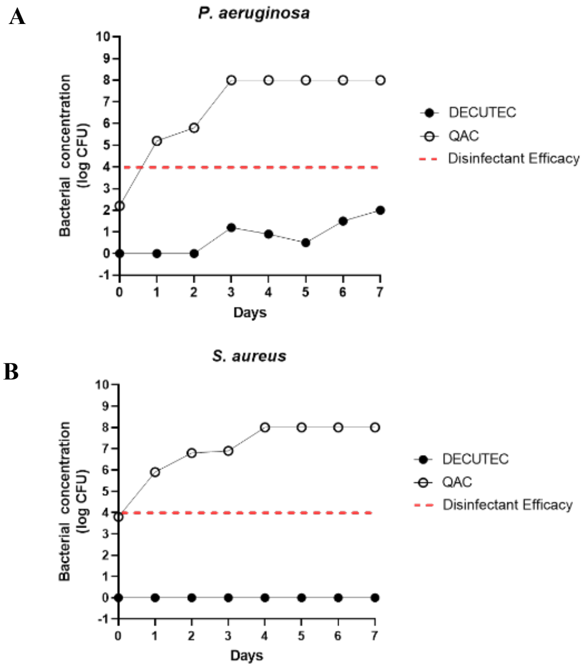

Figure 1: Antibacterial activity over time (log cfu/mL) of DECUTEC and a Quaternary ammonium compound (QAC) against *P. aeruginosa* (A) and *S. aureus* (B).

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Electro-Flexure Response of Multi-Functional Natural Fiber Hybrid Composites

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Abstract:
An experimental study was conducted to investigate the electro-flexure response of conductive natural fiber hybrid laminate composites. The composites were composed of laminates of jute and flax fibers, and the composites were subjected to flexural loading for the electrical and bending response. Multi-walled carbon nanotubes were shear mixed and ultrasonicated into the epoxy matrix. Short carbon fibers were reinforced in-between the laminates using "wet flocking" technique. To measure the electrical response under flexural loading, a four-point circumferential probe method was used. A parametric study was conducted to investigate flexural performance and damage sensing by varying carbon fiber lengths (150 and 350 µm) and the carbon fiber densities (500, I 000, 1 500, and 2000 fibers/mm^2 . The addition of carbon fibers decreased the flexural strength for most of the cases, however increased the flexural strain at break for all composites of carbon fiber length of 150 µm. During the nonlinear deformation, the composites of carbon fiber length of 150µm demonstrated a linear increase in resistance; however, that of carbon fiber length of 350 µm showed increasing slope of resistance. Overall, the composites of carbon fiber length of 350 µm showed lower resistance change at break compared to that of carbon fiber length of 150 µm.

Keywords: Hybrid natural fiber composite, electro-flocking. multi-functional, damage detection, flexural strength

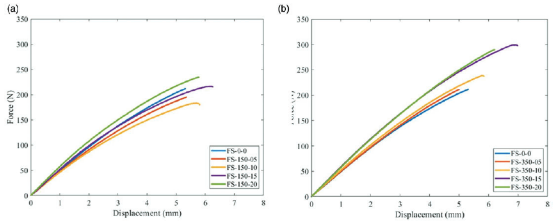

Figure 1: The characteristic force-displacement curves for: (a) FS-150-XX series and (b) FS-350-XX series.

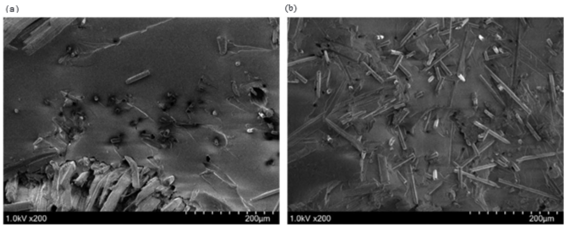

Figure 2: Scanning electron microscope image of: (a) FS-1SO-I000 and (b) FS-350-1000.

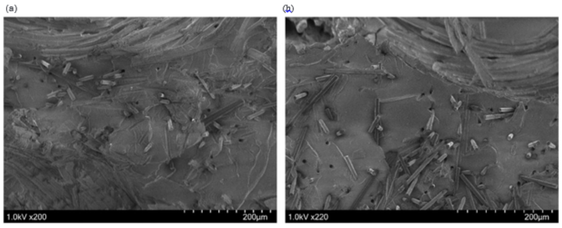

Figure 2: Scanning electron microscope image of: (a) FS-350-500 and (b) FS-350-2000

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Synthesis of porous high-temperature superconductors via a templated approach

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Abstract:

Conventional syntheses of high-temperature superconductors involve standard solid-state techniques, where solid precursors are ground and pressed into pellets prior to calcination. These techniques can result in poor purity of the product, along with little to no control over its nanostructure. Cuprate high-temperature superconductors such as $YaBa_2Cu_3O_7$ and $Bi_2Sr_2CaCuO_8$ can exhibit poor superconductivity at grain boundaries, so control over the nanostructure can be integral to optimise their properties.[1] Synthesis of a porous superconductor could yield interesting properties – such as enabling rapid cooling through submersion directly into the cryogen, and shorter oxygen annealing steps due to the high porosity creating shorter diffusion paths for the oxygen.[2,3] Melamine formaldehyde sponges are available commercially as the 'Magic eraser' and exhibit 99 % porosity.[4] These foams have not yet been explored as templates for high-temperature superconductors, so their effectiveness as a template is assessed in this work.

In this talk, we assess three different methods of using melamine formaldehyde as a sacrificial template in the sol-gel synthesis of $YaBa_2Cu_3O_7$ and $Bi_2Sr_2CaCuO_8$. These methods involve: using the sponge with an aqueous solution of constituent metal nitrates; first coating the sponge in sodium alginate, before soaking the sponge in metal nitrate solution; and a modified Pechini method, where ethylene glycol and citric acid are used to gel around the sponge. We analyse each method's effectiveness at replication of the sponge's morphology by scanning electron microscopy, and the purity of the final product through powder x-ray diffraction and Rietveld refinement.

Keywords: high-temperature superconductivity, Bi-2212, Y-123, porous material, templated synthesis, sol-gel synthesis,

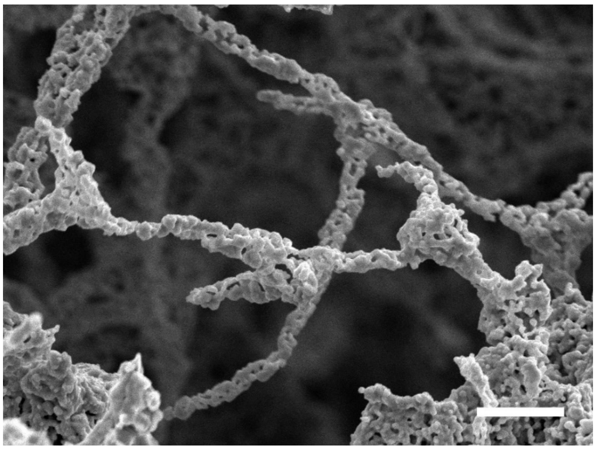

Figure 1: Scanning electron micrograph depicting the morphology of the $YaBa_2Cu_3O_7$ sponge. Scale bar indicates a length of 10 µm.

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From solution to surface: Molecular engineering of functional supramolecular assemblies on graphene-based surfaces

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Abstract:

Applying supramolecular chemistry principles to functionalize graphene for photonic applications[1] is a challenge because not only graphene can quench the emission from adsorbed molecules, but the functional units also need to be placed at a certain distance in order not to interfere in their functionality. We decided on a design based on molecular dyads, composed of a pedestal and a chromophore, connected in a way that the emissive component stands up, and induce self-assembly in the pores of a 2D network previously arranged on the surface. The 2D network consisted of interdigitated 1,3,5-tristyrilbenzene (TSB) molecules terminated by alkoxy peripheral chains containing 12 carbon atoms which form an ordered array of pores with a diameter of 1.3 nm assuring the lateral distancing of the functional units[2]. In this work we tried to understand how the properties of molecules in solution can be transferred to a surface by studying two assembly strategies. In the first we started by assembling the dyad consisting in a zinc phthalocyanine (ZnPc) and a perylenetetracarboxylic diimide, as the emissive component in solution and then let the preassembled dyad fill the pores of the host-guest template on graphene. These components can form two-types of dyads, depending on the supramolecular interactions that dominate the equilibrium in solution, "metal-ligand" and "π-π stacking" dyads. In our second approach we first filled the pores with the zinc phthalocyanine pedestal and then exposed the latter to the perylenetetracarboxylic diimide. In both cases the structures obtained were studied by scanning tunneling microscopy and x-ray photoelectron spectroscopy. We found that ZnPc molecules are mostly associated with the BPDI4 molecules via metal-ligand coordination by depositing one building block after another.

Keywords: Supramolecular self-assemblies, graphene, surface functionalization, zinc phthalocyanine, STM, XPS,

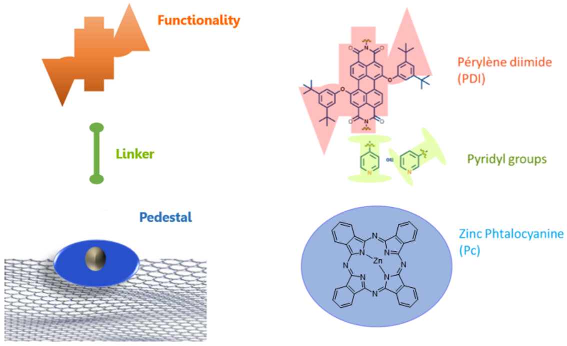

Figure 1: llustration of the rational design to integer and organize a functional building-block on graphene.

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Ionic concentration and substrate dependent surface potential of single layer graphene by in-liquid Dual-Harmonic KPFM

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[2] Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee , USA
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Abstract:

Due to its unique properties – electrical, optical, mechanical and chemical-, graphene is nowadays investigated as the active element in electronic devices to be used in a range of applications, including the biomedical field[1,2]. When being part of a device working in a biological ambient, graphene is in contact with an electrolyte that may affect its electronic properties. Therefore, understanding the charge modulation of graphene in a liquid environment is key to move towards an improved technology and device functionality.

Kelvin probe force microscopy (KPFM) is a powerful technique capable of locally measuring electronic properties with high spatial resolution and, thus, providing unique spatially-encoded information: surface potential distribution along a device, tuning of the work function and quantitative measurement of electronic parameters such as capacitance over a surface, etc. In this work, we use a particular KPFM-based technique, dual-harmonic-KPFM (DH-KPFM)[3], to measure the work function of chemically-grown single layer graphene, deposited on different substrates, in contact with an aqueous electrolyte to evaluate its dependence on the electronic nature of the substrate, the pH and the ion strength of the electrolyte. Other techniques such as Raman spectroscopy, electrochemical impedance spectroscopy, X-ray and ultraviolet photoelectron spectroscopy complement the experimental work, providing information about graphene's doping level and its dependence on the ionic environment and the substrate; furthermore, we will also discuss the effect of chemical residues present on the graphene surface.

Our findings indicate that adsorbed charges on the surface of graphene, resulting from contamination of the fabrication process, play a key role in graphene´s charge modulation. Additionally, distinctively behaviour of graphene's capacitance when supported on conductive and insulating substrates is observed whith pH and ionic concentration changes. Last, our measurements prove the capability of the in-liquid DH-KPFM as a tool for the obtention of the workfunction of graphene in low ionic electrolyte concentrations.

Keywords: graphene, electronic properties, workfunction, KPFM, DH-KPFM

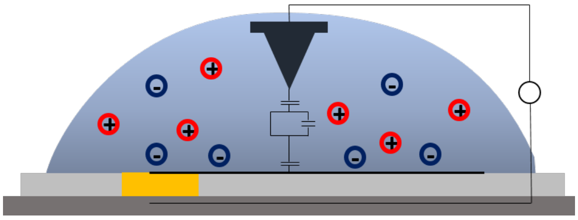

Figure 1: Schematic representation of the experimental set-up employed in this work: DH-KPFM enables the measurement of the sample surface potential by applying an AC voltage to the AFM tip acquiring the amplitude response of the first and second harmonic electrostatic force and the combination of them.

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Submicron 4D Printing of Shape Memory Polymer

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Abstract:

Four-dimensional (4D) printing refers to 3D printed structures that exhibit a response to time. Notable demonstrations are predominantly of macroscopic shape-changes enabled by stimuli-responsive materials triggered by temperature, humidity, light etc. While changes in shape with applications in self-folding and gripping structures have been achieved, changes in visual appearance due to structural colours have been hindered by the limited resolution of the printed features. Here, we present probably the first results of 4D printing at sub-micrometre dimensions. Doing so extends its applications to nanophonics, as the structures are now sub-wavelength in dimension. We formulated a shape memory polymer photoresist based on Vero Clear and achieved submicron scale 4D printing features (with feature size of ~300 nm) by two-photon polymerization lithography (TPL). To demonstrate our submicron 4D structures and their shape memory effect, a 4D structural colour print consisting of a square grid exhibiting different colours was designed and fabricated. A schematic of this structure is shown in Figure 1. When compressed, the device loses its colours as the structures are flattened. Remarkably, due to the shape memory effect, the original surface morphology of the nanostructures recovers along with its optical properties, when heated above the transition temperature. Our high-resolution 4D printing and its excellent reversibility in both microtopography and optical properties could be a promising platform for temperature-sensitive labels, photonic devices and on-chip applications.

Keywords: 4D printing, two-photon polymerization lithography, shape memory polymer, programmable colour generation

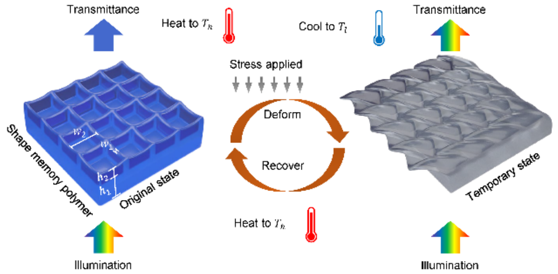

Figure 1: Schematic of sub-micron 4D printing using in-house shape memory polymer resin. The as-printed structures exhibit structural colour due to the interaction between the structure and the visible light. Deforming the structure at a high temperature (higher than the glass transition temperature, T_g) and removing the stress at room temperature freezes the structure in a flattened state where it is colourless. Heating to T_g recovers the as printed structure as well as the structural colour.

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3D Printed Colorful Vortex Beam Generator and Decoder

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Abstract:
As a fundamental property of light, the orbital angular momentum (OAM) of light was discovered in the Laguerre-Gaussian beam in the 1990s. To date, the vortex beam is generated by coherent laser or partial coherent source. However, what would one achieve if white light were used instead? Here, we report a 3D printed optical element to achieve colorful optical vortices from halogen lamp. Furthermore, we demonstrate the use of colorful vortex beams in pairwise optical authentication, thus introducing a new form of physical-digital encryption.

Keywords: orbital angular momentum, white light, two-photon polymerization, color printing, optical authentication.

Optical vortices provide promise in increased information capacity in optical communication and has been applied in super-resolution microscopy and lithography. Currently, the orbital angular momentum (OAM) of light is attracting more and more attention in optical information transfer, super-resolution imaging, and light-matter interactions, etc. However, the generation of such optical vortices requires coherent laser source, which limits its application in 3D display and optical metrology. White lights are readily available and potentially allow for compact and simpler implementation for the next generation of virtual reality display and optical authentications[1]. Here, we have a systemetic study on generating colorful optical vortices under white light thermal source and fabricating the colorful vortex beam (CVB) unit with the nanoscale two-photon polymerization 3D printing technology.

The CVBs are generated by incorporating the spectral modulation of nanopillar structures with the phase modulation of a converging spiral phase plate in a single element. The addition and subtraction of the topological charges in colorized OAM of light are discussed in both real and momentum space. Our CVBs are systemaically studied both in simulations and experiments, paving the way for multidimensional light modulation and decoding directly under white light illumination. In addition to the spectrum and OAM dimensions, spatial modulation of the incident white light can be also achieved by arranging our CVB units at specific positions discretionarily.

The CVB unit (Fig. 1(a) inset) is fabricated using two-photon polymerization 3D printing technique, with a customized script to control the convering and spiral surface accurately. To accelerate the printing, we developed a method of two-density three-step nanoscale 3D printing. At first, the inner part of the CVB unit is fabricated with relatively large slicing and hatching distances. Then, the top surface of the CVB unit is fabricated with finer parameters and slower writing speed to achieve a smoother surface. At last, the nanopillars are added onto the surface in the order of coordinates as the function of a color filter. By adjusting the surface tomography and heights of nanopillars, we can arbitrarily control the focallength, color, and tological charges of the colorful optical vortices[2].

As a potential application of colorful optical vortices, we developed a pairwise authentication scheme based on our CVB units, which is inspired by the tiger tally pair (~B.C. 2300 Chinese authentication token pairs) holding multiple complementary features. Beyond ancient tiger tally and conventional optical security labels, our photonic tally pair holds the advantages of reciprocity and one-to-may matching and validation scheme, capable of realizing mutual optical validation and cross optical validation. The color elimination and annihilation of topological charges at corresponding spatial positions provide subtractive and complementary features for the design of next-generation optical anticounterfeiting devices. Our colorful optical vortices enable OAM generation with broadband white light, which could find potential applications in anti-counterfeiting, optical metrology, high-capacity optical encryption, and on-chip 3D photonic devices.

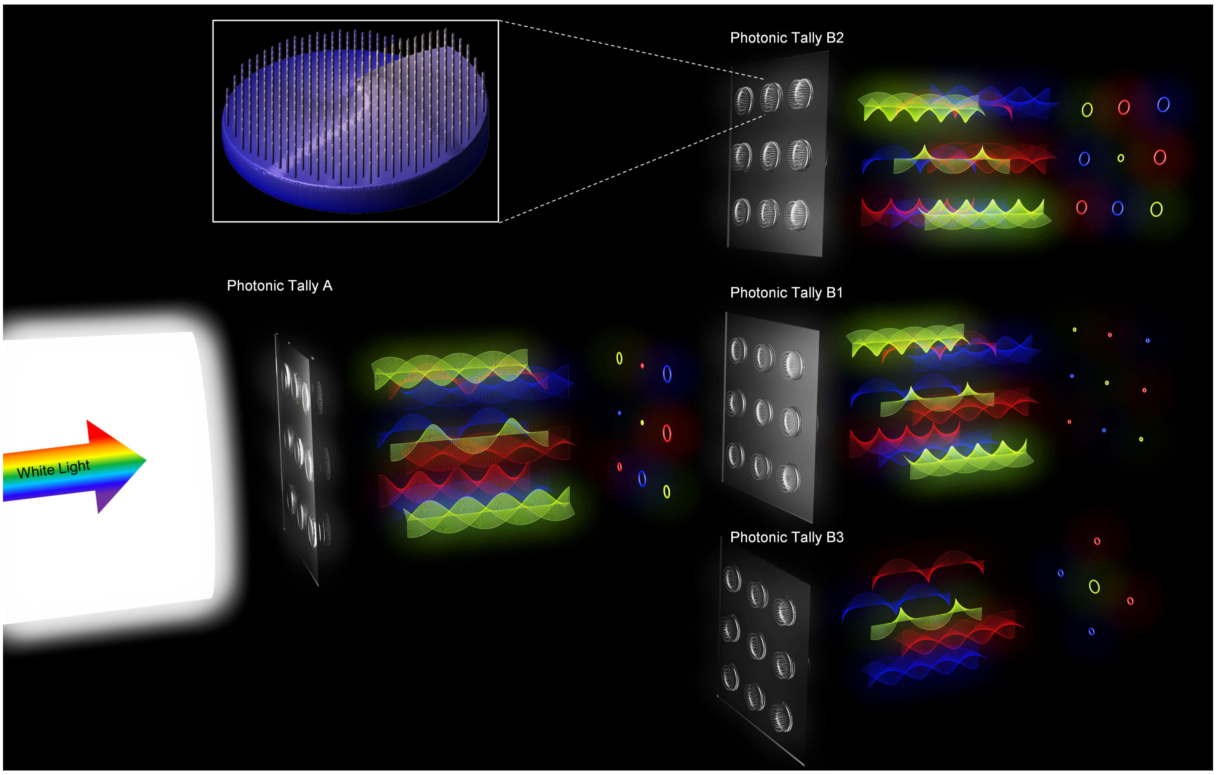

Figure 1: Schematic of a photonic tally pair operating with white light. With a single Photonic Tally A, multiple distinct colorful vortex beams (CVB) can be realized through different pieces of Photonic Tally Bs. Digital readout of these resulting optical patterns enable secure pairwise optical authentication.

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Nanoscale 3D Printing of Light Field Prints

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Abstract:
Under white light illumination, a light field print (LFP) displays three-dimensional (3D) information that is perceived by an observer. This 3D information can be perceived by the naked eye and does not require wearing of special glasses. Changing perspectives of a 3D image are perceived by the observer from varying viewing angles. However, conventional LFPs have the problem of limited resolution and misalignment between their lenses and colour pixels. Here, we use nanoscale 3D printing to directly fabricate LFPs out of transparent resin in a single patterning step that automatically solves the alignment issue. This approach also produces simultaneously high spatial resolution (29–45 μm) and high angular resolution (~1.6°) across 15 × 15 views. We show that a single nanopillar ~300 nm diameter suffices as a colour pixel of the LFP. Our work signifies a step towards hyper-realistic 3D images and security tags for high-value goods.

Keywords: Nanophotonics, 3D printing, light field, security applications

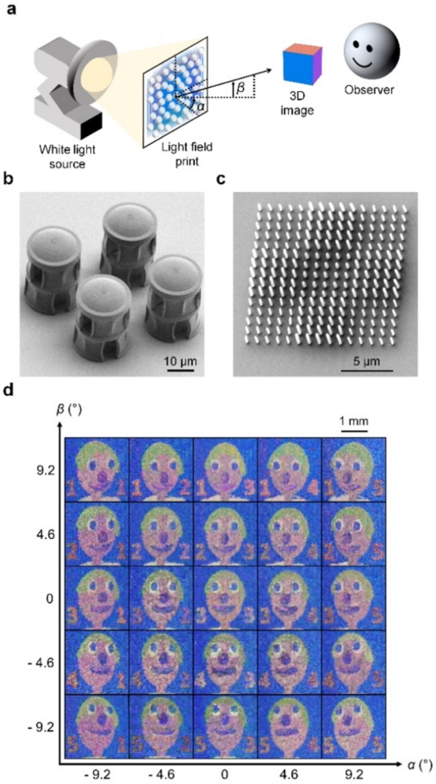

Figure 1: (**a**) Schematic of how a light field print (LFP) works. A white light source illuminates the LFP in transmission mode, which then projects a 3D image to the observer standing at the viewing angle (α,β). (**b**) Scanning electron microscope image of 4 display units in the LFP. Each display unit comprises a lens, a supporting tower and a block of pixels underneath the lens. (**c**) Scanning electron microscope image of nanopillar pixels under each display unit. (**d**) Digital camera photographs of a light field print captured from varying viewing angles (α,β).

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Effect of Nano Silica on Mechanical and Water absorption properties of Hybrid composites of Basalt fibers, Glass fibers, Hemp fibers and Unsaturated Polyester Resin

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Abstract:
Present work presents, Unsaturated Polyester Resin (UPR) composites with an optimum weight percentage of Basalt fibers (BF), Glass fibers (GF), Hemp fibers (HF) and hybridization of Basalt fibers with Glass (BG) and with Hemp (BH). The effect varying concentration of of Nano Silica viz 1,2,3,4,5 weight percent on properties of optimized inorganic fiber reinforced UPR composites obtained by Vacuum Assisted Resin Infusion (VARI) technique. The effects of different type and concentration of fibers, hybridization and percentage of Nano Silica on Mechanical Properties (Tensile, Flexural, Izod Impact and Hardness) and Water absorption characteristics of composites are investigated and discussed. The maximum tensile strength and Tensile Modulus were found for UPR+BF+2% Nano Silica (316.5 MPa & 11.29 GPa, respectively). The hybrid composites showed intermediate results between the neat fibers composites. It was found that all the mechanical properties were enhanced till 2% Nano Silica loading, and after that, the values started declining. Water absorption behavior was studied till the water uptake percentage attained a constant value, and it was found that equilibrium water uptake decreased till 3% of Nano Silica loading. The fractured surface of the composites was studied for fiber pull out, fiber breakage, interface and uniformity using Scanning Electron Microscopy (SEM).

Keywords: Polymer-Matrix Composites, Basalt Fibers, Hybrid Nano composites, Glass fibers, Hemp fibers, Mechanical Properties.

The investigation of cathode layer of Molten Carbonate Fuel Cell manufactured by using printing techniques

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Abstract:
The paper presents an investigation on the three various cathode layers for Molten Carbonate Fuel Cell obtained by using printing techniques. The main difference during manufacturing process was a substrate used during printing the layers. There were glass, and two different papers. The cathodes were investigated by both experimental as well as theoretical attempts.

Table I:

	$\delta_{cathode}$, mm	$\sigma_{cathode}$, S/cm
1708-SMa14	0.895	0.0270
1708-TLMa12	0.95	0.0217
1708-TLMa13	0.87	0.0172

Based on experimental data, the influence of a given cathodic layer on the fuel cell performance were tested, the results of approximation of experimental data using a mathematical model allow to estimate the conductivity of given layers. The results are summarized in the Fig. 1.

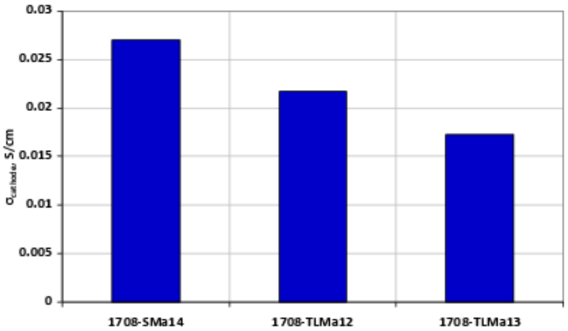

Figure 1: Estimated conductivity values of the tested cathode layers

The largest conductivity was achieved by the cathode 1708-SMa14, which was produced by screen printing on a glass substrate.

The cell containing the printed cathode 1708-TLMa12 was characterized by the lowest power density under reference conditions (with and without CO_2 at the anode). Fuel cells containing cathodes 1708-TLMa13 and 1708-SMa14 had comparable power densities for reference conditions without CO_2 at the anode (they would probably also have comparable densities for reference conditions, as overall results between the reference (with CO2 at anode inlet) and without CO2 at anode inlet did not differ significantly).

In the case of maximum flows (MaxFlow), the cell containing cathode 1708-SMa14 had the best results (both in the case of current-voltage curves and power density). In this case, fuel cells containing cathodes 1708-TLMa12 and 1708-TLMa13 had comparable results. However, this is the case in which the cell's power is greater at the expense of its efficiency.

The poorer performance of the fuel cell containing the printed cathode 1708-TLMa12 could be due to a lower average operating temperature compared to the other two cells. Nevertheless, the mathematical model of the fuel cell that takes into account the influence of temperature on performance, eliminating this disruption, was used to assess this phenomenon.

The results of experiments showed that using printing methods one can obtain working elements of molten carbonate cells with similar conductivity of cathodes (σ, S/cm). The best results were obtained for a cathode made by screen printing on a glass substrate.

Acknowledgments
The project is co-financed by Polish National Center for Research and Development of Operational Programme Smart Growth, INNOCHEM sectoral programme granted by agreement number POIR.01.02.00-00-0045/16.

Keywords: fuel cells, molten carbonate fuel cell, printing technologies

Nanotech / NanoMetrolgy joint session I.B: Nanomaterials Modelling and Characterisation

TEM and related microanalytical techniques: a powerful tool for the characterization of low band-gap rod-coil block copolymer:PC61BM blend water-processable nanoparticles

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Abstract: The assembly of hydrophobic conjugate polymers into water-processable nanoparticles represents an innovative technology with many applications in optoelectronics, biology, and medicine. Our studies are based on different amphiphilic low band gap rod-coil block copolymers (LBG-BCPs) composed by a rigid hydrophobic p-type semiconductor polymer, PCPDTBT, and 4-vinylpyridine-based (4VP-based) coil block that interacts with water and has different molecular structure and length for each BCP used. Exploiting the BCP structure and characteristic we synthesized stable WPNPs in water by mean of an adapted miniemulsion approach. The presence of the 4VP-based coil makes the WPNPs stable in water. To prepare a material for OPV device active layer, we mixed the LBG-BCPs with an electron acceptor fullerene derivative ([6,6]-phenyl-C$_{61}$-butyricacid methyl ester, PC$_{61}$BM) to achieve blend WPNPs (b-WPNPs). The WPNPs and b-WPNPs were fully characterized by TEM, STEM-EDX, EFTEM, AFM, and DLS and z-potential [1,2,3].

The Transmission Electron Microscopy and the micro-analytical technique connected are fundamental to provide information about morphology, elemental intraparticle distribution with nanometric resolution (STEM-EDX analysis), which allows to understand how the LBG-BCPs autoassemble to give WPNP. Moreover, an application of the EFTEM images based on the plasmon peak signal is demostred to be fundamental to identifie in the b-WPNPs the PCBM-rich areas and the acceptor-rich domain shape, allowing to correlate the PC$_{61}$BM distribution inside the WPNP with the material efficiency [3,4,5].

Keywords: amphiphilic low band gap rod-coil block copolymers, Water processable nanoparticle,Transmission electron microscopy, EDX, EFTEM

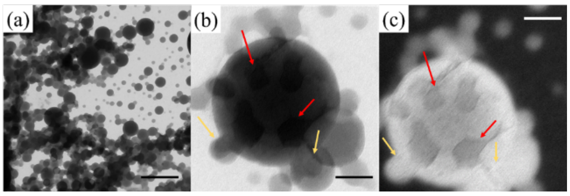

Figure 1: 1 BF-TEM images of the a) BCP5:PC$_{61}$BM (1:3) blend NPs, b) detail of one blend nanostructure, and c) corresponding EFTEM image. The scale bars are (a) 500 nm and (b,c) 50 nm, respectively. Red and yellow arrows emphasize the differences observed between BF-TEM and EFTEM images.

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Ethics of Nanotechnology in the framework of the NanoFabNet Hub for sustainable, industrial-scale Nanofabrication

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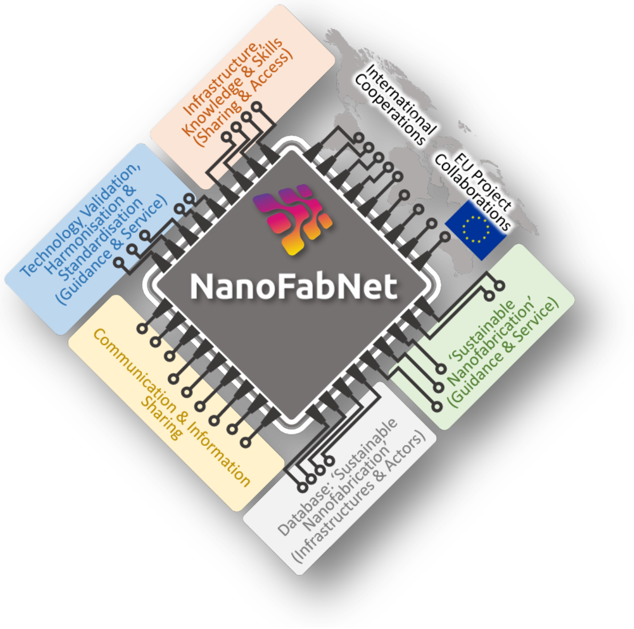
Abstract:

NanoFabNet (https://nanofabnet.eu/) has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 886171. The NanoFabNet project aims at creating a strong international Hub for sustainable nanofabrication (in terms of human health, ethics, environment, life cycle analysis, …) that stands for (a) a well-implemented, guided approach to high levels of safety and sustainability, (b) trusted technical reliability and quality, and (c) compliance with and drive of harmonisation, standardisation, and regulation requirements, amongst all of its members and along the nanofabrication value chains.

The NanoFabNet Hub (https://nanofabnet.net/) is expected to provide the following services: creation of a NanoFabNet brand to improve confidence in products and technologies resulting from nanofabrication; identification and access to proper databases related to key players/infrastructures, initiatives & networks at national, European and international levels (processes, platforms, methodologies, sustainability, risk assessment tools, metrology, standardization, tools for ethical assessment and for dialogue with civil society, etc.); technology validation (validation/labeling guides and services, organisation of proficiency testing, etc.); facilitation of access to infrastructures; communication and information sharing (regulations, technologies, standardisation, good practices, etc.); international cooperation (USA, China, Japan, Australia ...) and promotion of European projects; identification of the needs in the field and establishment of roadmaps to feed European strategy.

The presentation will give an insight on the main features of the NanoFabNet Hub, and will make a particular focus on the ethical concern related to nanotechnology. Due to the generic and enabling nature of nanotechnology and nanofabrication, and the diversity of their applications and possible impacts (be it in medicine, in ICTs, in materials, etc.), nanotechnology and nanofabrication are involved in a array of societal and ethical issues dealing with privacy, autonomy, social divide, environmental justice, human enhancement, etc. The revolutionary promises and the problematic social expectations (such as “transhumanism”) sometimes associated to them since the early stages of their development, have also importantly shaped the public debate on nanotechnologies, and even aroused a social mistrust and a strong social opposition to them in some countries (the reluctance to Covid19 vaccines being a recent example of them). We will discuss the best way to succeed in the upstream identification of the ethical issues in nanotechnology development, and to involve researchers, industry and civil society in ethical reflection to enable the harmonious development of nanotechnology.

Keywords: sustainable nanofabrication, international Hub, stakeholders, validation and harmonisation, ethical impact assessment, public trust.



Length and diameter determination of rod-like nanoparticles using Depolarized Dynamic Light Scattering

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Abstract:

Anisotropic nanoparticles, such as nanorods, nanodiscs, etc. are widely used in application fields such as medicine (fluorescent enhancers, tumor markers,etc.), electronics (molecular electronic devices, sources of local heating) for example. In particular, metallic nanorods exhibit promising optical, electrical and magnetic properties due to the plasmon resonance. Since SPR effect is closely related to the particle geometries, being able to monitor their shape and size at different stages of their synthesis turns out to be critical for these applications.

Here we described a patented optical set-up combined with a data analysis method for performing Depolarized Dynamic Light Scattering (DDLS)[1]. This method is derived from the well-known DLS technique and provides a reliable measurements of the rotational diffusion coefficient D_r along with the translational diffusion coefficient D_t of analysed anisotropic particles[2]. This is made possible by the use of a vertical polarized incident light and a detection arm mounted on a goniometer covering a continuous wide range of scattering angles. The light detector is equipped with a specific polarizer allowing to select either vertically polarized (v-v) or horizontally polarized (v-h) scattered light on two separate channels (see Figure1).

The experimental determination of D_r and D_t gives then access to the calculations of lengths and aspect ratios of nanorods thanks to the use of an appropriate hydrodynamic model.

Several gold nanorods, having lengths below 60 nm and aspect ratios between 2 and 6, have been either obtained commercially or synthesized according to literature,[3] and analysed using this approach. The results show very consistent sizes as compared to transmission electron microscopy observations, as the maximum deviations don't exceed 15% for the lengths and 20%. The discrepancies between DDLS and TEM arising presumably to size and shape polydispersity.

Keywords: Depolarized Dynamic Light Scattering, DDLS, multi angle DLS, anisotropic, particle shape, nanorods.

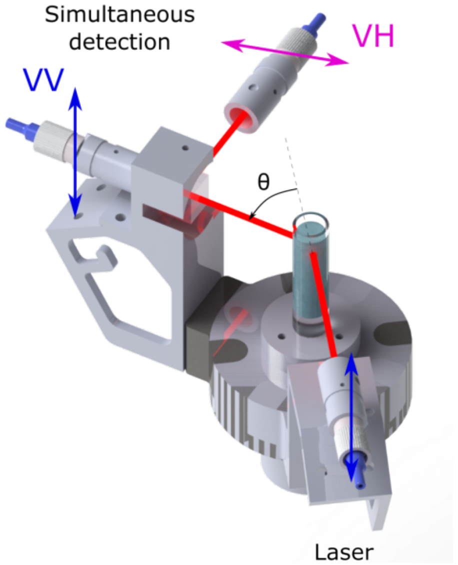

Figure 1: Scheme of the DDLS instrument optical setup. The vertical polarized incident light is scattered by the susepion of anisotropic nanoparticles before being detected simultaneously by two detection channels. The scattering vector is selected by adjusting the θ angle of the goniometer. Both channels are equipped with polarizers selecting either vertically polarized (v-v) or horizontally polarized (v-h) scattered light.

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A Unique And Enhanced Approach To Measure The Effective Surface Tension Of A nanoparticle coated Liquid Marble

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Abstract:

A liquid marble is a non-wetting droplet encapsulated with micro-or nano-sized particles. Distinctive properties of a liquid marble such as low evaporation rate, low friction, and tunable porosity of the shell enable it to be a convenient tool for microfluidic applications. Recently, the fundamental research work on liquid marble focuses into understanding its stability, robustness, and effective surface tension. These key properties are inherently related to the structure and properties of the liquid marble shell. A liquid marble shell consists of encapsulating particles and the air pockets. The structure and the properties of the liquid marble shell depends on the properties of the encapsulating particles and the liquid marble preparation method. For an instance, effective surface tension values of liquid marbles prepared with encapsulating particles of different properties, are inconsistent. With the growing interest of liquid marbles in digital microfluidics, it is important to understand the factors for the inconsistent effective surface tension values and how such inconsistencies can be diminished. A major contributor to the inconsistent effective surface tension values could be the liquid marble preparation method. The most popular liquid marble preparation method is rolling a droplet on a hydrophobic powder bed. Scientists prefer rolling method as this is faster and more convenient. However, a manual preparation method doesn't consider the rolling parameters such as the duration of rolling or rolling speed. The lack of control over the rolling parameters could result in the inconsistent effective surface tension values of a liquid marble. A systematic approach to prepare the liquid marbles, where the rolling parameters are kept constant should address the abovementioned issue. In this work, we are the first in i) determining the effective surface tension of a liquid marble utilizing its natural oscillation and ii) investigating the effect of the preparation methods on the effective surface tension values of a liquid marble. We used a high non-uniform DC electric field to generate the dieletrophoresis force to oscillate the liquid marble at its natural frequency. Our method does not require contact angle measurement which is troublesome incase of a liquid marble. We compare the effective surface tension values determined by natural oscillation of the liquid marbles prepared by various preparation methods. We found that the effective surface tension values of the liquid marbles prepared manually are inconsistent. A systematic preparation method using a vortex mixer at a constant rolling speed significantly enhances the consistencies of the effective surface tension values. Nevertheless, an excessive rolling speed causes interfacial jamming at the liquid marble shell and reduces the uniformity at the liquid marble shell. Such phenomenon at the liquid marble shell is responsible for the inconsistent effective surface tension values at higher rolling speed.

We believe our work could provide a new insight into the effective surface tension of a liquid marble, which could help digital microfluidics community. Overall, it solves the long-standing problem of inconsistent effective surface tension of liquid marble-based technology

Keywords: Nnaomaterials, Liquid Marble, Oscillating drop, Effective surface tension, Interfacial jamming

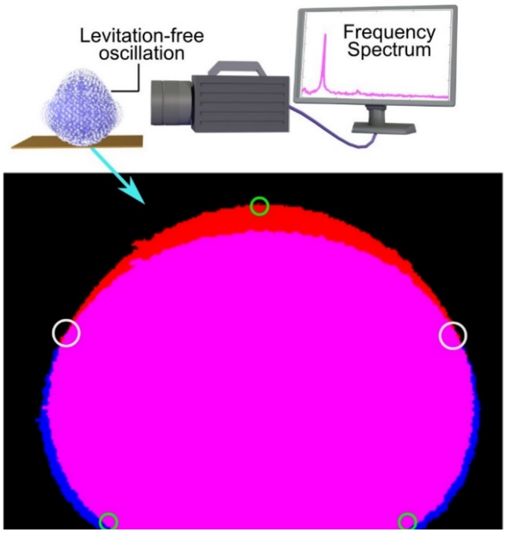

Figure 1: Figure illustrating the fundamental question that we are tempting to solve experimentally: what is the importance of silica surface modification nanoporous silica-based sol-gel glasses prepared from functionalized

organosilane precursors on the parameters affecting the conformation, biological activity and functionality of encapsulated biomolecules.

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Experimental characterization and numerical modelling of polymer-based nanocomposite properties

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Abstract:

The need of the aerospace industry to employ lighter and more efficient components for aircraft, satellite, and launcher structures has led to an ever-increasing development of innovative materials like composites and nanocomposites [1]. Among them, polymer-based composites reinforced with nanoscale reinforcements have recently attracted the interest of the academic and industrial communities, since the addition of low concentrations of nanofillers results in enhanced mechanical, thermal, and barrier properties [2]. The increase of the reliability and efficiency of these materials requires a proper understanding of their properties. In this work, a chemical characterization of samples composed by an epoxy resin nanomodified through the addition of different inorganic nanoparticles is carried out through FTIR Spectroscopy and X-Ray Diffraction, and a Thermogravimetric Analysis (TGA) is performed to analyse the effect of the different nanomodifiers on the thermal degradation of the resins. The microanalyses of the samples are performed by Environmental Scanning Electron Microscopy (ESEM), and their morphologies are studied by Transmission Electron Microscopy (TEM) (see Figure 1). Tensile and fracture tests are also carried out to study the effect of the different nanomodifiers on the overall stiffness and fracture toughness of the resins, respectively. As for the numerical modelling, a peridynamic (PD) model is implemented to estimate the effective tensile modulus of the different nanocomposites [3]. The newly developed approach models randomly distributed nanofillers with different shapes and orientations and simulates interphase properties and nanofillers agglomerations. The fracture toughness of the nanomodified resins is instead studied through a classical continuum mechanics-peridynamics coupling strategy [4]. Comparison to experimental data confirms the capability of the PD model to accurately reproduce the effective stiffness of the different nanocomposites and of the coupling approach to properly model their fracture properties.

Keywords: Polymer-based nanocomposites, Inorganic nanoparticles, Thermal characterization, Chemical characterization, Electron Microscopy, Mechanical Testing, Peridynamics, Classical continuum mechanics-Peridynamics coupling.

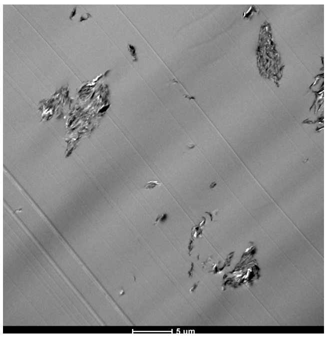

Figure 1: TEM image of an epoxy resin nanomodified through the addition of 3% wt of inorganic nanoparticles. The micrograph shows the coexistence between resin-rich areas and nanofiller-rich regions with intercalated and phase-separated morphologies. Some partially exfoliated tactoids are also identifiable.

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Quantification of the Total and Accessible Number of Functional Groups and Ligands on Nanomaterials

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Abstract:

Surface-functionalized organic and inorganic nanoparticles (NP) are of great interest in the life and material sciences, as they can be used e.g. as drug carriers, fluorescent sensors, and multimodal labels in bioanalytical assays and imaging applications. NP performance in such applications depends not only on particle size, size distribution, and morphology, but also on surface chemistry, i.e. the total number of surface functional groups (FG) and the number of FG accessible for subsequent functionalization with ligands or biomolecules, which in turn determines surface charge, colloidal stability, biocompatibility, and toxicity.[1] Methods for FG quantification should be simple, robust, reliable, fast, and inexpensive, and allow for the characterization of a broad variety of nanomaterials differing in size, chemical composition, and optical properties.

Aiming at the development of simple, versatile, and multimodal tools for the quantification of many bioanalytically relevant FG such as amine[2,3], carboxy[2,3], thiol and aldehyde[4] functionalities, we investigated and compared various analytical methods commonly used for functional group quantification (Figure 1). This includes electrochemical titration methods, dye-based optical assays, and other instrumental analytical techniques such as nuclear magnetic resonance, mass spectrometry, and thermal analysis methods.

Keywords: functionalized nano- and microparticles, particle surface analysis, surface group quantification, terminal functional groups, optical assays.

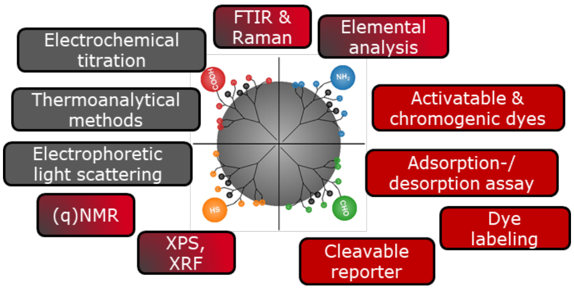

Figure 1: Overview of analytical methods commonly used to quantify the total number of FG (grey) and accessible number of FG (red) present on the NP surface.

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Microfluidics and Microscopy – A Powerful Combination for the Development of Novel Micro-and Nano-structured Soft Materials with Designer Functionality

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Abstract:

Conjugated polymer materials have recently been extensively investigated in diverse areas ranging from opto-electronics to life sciences.[1] In relation to photonics applications, the use of whispering gallery mode micro-resonator approaches has given rise to an impressive variety of micro-structure enabled communications and sensing device prototypes.[2] The fabrication of micro-resonators is a demanding task in terms of reproducible production of structures that possess the necessary composition, geometry, dimensions and interface smoothness.[3]

In this regard, using real-time *in situ* (on-chip) optical imaging methods, we developed a T-junction microfluidic droplet generation technology for the production of conjugated polymer micro-particles. MEH-PPV, a polymer semiconductor material was selected. We studied MEH-PPV/$CHCl_3$ droplet formation systematically varied parameters, to identify effects on MEH-PPV micro-sphere morphological and spectroscopic properties. Imaging studies based on optical microscopy, field emission SEM were extensively employed for morphology characterisation and data were combined with spectroscopy data to build a comprehensive process-property map for this system.

By including additional components in the organic phase, the microfluidic approach was extended to the formation of biphasic 'Janus' or 'snowman' microparticles composed of emissive MEH-PPV and biocompatible, biodegradable PLGA as well as triphasic, 'multi-lobed' PLGA-MEH-PPV-PLGA micro-particles that were extensively characterised using a novel correlative confocal fluorescence-SEM method. Further incorporation of superparamagnetic oleic-acid stabilised Fe_3O_4 nanoparticles permitted the formation of magnetic field-responsive fluorescent MEH-PPV-PLGA Janus particles that behaved as a type of active matter that exhibited magnetic field-induced liquid-solid extraction and other dynamic phenomena, such as, field-assisted single-particle lateral translocation and dipole-mediated multi-particle chaining both of which were monitored during real-time *in situ* imaging studies.

The as-prepared polymeric multi-functional spheres with unique asymmetric structures and properties offer promising abilities to a wide variety of applications such as target drug delivery, bioimaging, and photovoltaics.

Keywords: conjugated polymer, droplet microfluidics, microscopy, spectroscopy, SEM, confocal, correlative characterization, Janus particle, iron oxide nanoparticles.

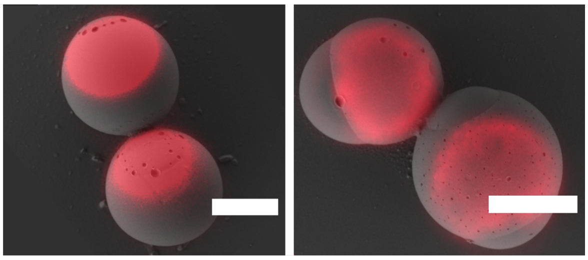

Figure 1. Correlative confocal fluorescence-SEM images of MEH-PPV-PLGA 'janus' and 'multi-lobed' micro-particles with nano-sized dimples on the MEH-PPV component. Scale bar: 5 μm.

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Physico-Chemical Characterization of Hydroxyapatite Nanoparticles from Tricalcium Phosphate Food Additive

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Abstract:

Tricalcium phosphate (TCP) is a commercially available product involved in numerous industrial applications such as in the food industry where it is used as a food additive (labelled E341). Since it was revealed in the United States that TCP food additive was composed of nanoparticles, the question of the presence of such nanoparticles in European products has become of interest to address consumer safety concerns. Here a physico-chemical investigation of three different TCP samples used in France and complying with European regulations is proposed (Figure 1).

X-Ray diffraction, Raman Spectroscopy, ^{31}P NMR as well as infrared spectroscopy revealed the main phase in the TCP samples to be hydroxyapatite (HA). The Ca/P molar ratio obtained by ICP-AES, which is characteristic of calcium phosphate compounds, is close to the 1.67 HA reference value. BET analysis of the N_2 adsorption-desorption isotherms provided specific surface area values consistent with the definition of nanomaterials. Transmission electron microscopy gave access to the morphology and overall size of the HA nanoparticles. The solubility determination in different pH conditions highlighted the persistency of HA nanoparticles in neutral and acidic conditions down to pH 3. Laser granulometry and zeta potential measurements respectively evidenced the agglomeration tendency of this compound in aqueous medium, whatever the pH value, and its negatively charged surface for pH conditions where dissolution is negligible (pH>5).

Finally, this study establishes a baseline for the definition of TCP food additive, which is composed of crystalline hydroxyapatite, similarly to observations made in the United States. In addition, all the TCP samples considered in this study contained very smalls objects with at least one dimension smaller than 100 nm, which is the main criteria for their classification as nanomaterials. Further work is under consideration to follow the fate of these nano-objects all along the gastro-intestinal tract.

Keywords: characterization, nanoparticles, tricalcium phosphate, food additive

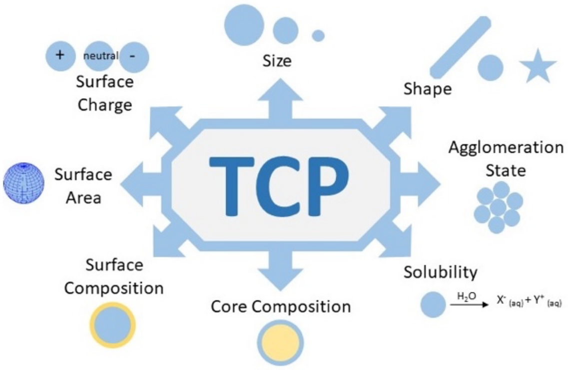

Figure 1: Figure illustrating the extensive characterization that TCP food additive entails as a nanomaterial

A simple approach to the deflection detection of the nanowires

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Abstract:

Nanowire (NW) research has transformed the research fields of electronics, sensors, energy harvesting and storage, drug delivery, wearable devices, and environmental applications. Central to the popularity of nanowire-based devices are their mechanical and electrical properties.

In recent years with the advancement of technology researchers were capable of fabricating pristine high aspect ratio NWs which are ideal for sensitive force and mass detection. It is promising to utilize these NWs as they are apt for detecting weak magnetic moments and force field gradients because of low stiffness and intrinsic mechanical losses at a wide temperature range [1]. We demonstrate a highly sensitive co-resonantly coupled cantilever sensor (figure 1) capable of detecting nanowire vibrations without the need for a dedicated setup since the coupled modes can be detected using the conventional cantilever deflection detection method. Co-resonance means matching the resonance frequencies of the individual sub-systems' flexural modes [2]. We quantify the mechanical properties of the NW and the coupled system by exploiting thermally generated mechanical fluctuations at room temperature. Then we present experimental evidence to prove that our coupled system conforms with the extensively discussed theoretical model of a coupled harmonic oscillator (figure 2). We exhibit a sensor with the advantages of easy detection of NW vibrations and a potentially highly sensitive magnetometry tool to study nanometer-sized magnetic particles. The simplicity of device fabrication and detection can be quite encouraging for the researchers who are to work on nanowire detection schemes and their applications.

Keywords: coupled cantilever oscillator, co-resonance coupling, signal enhancement, nanowire detection, sensitivity

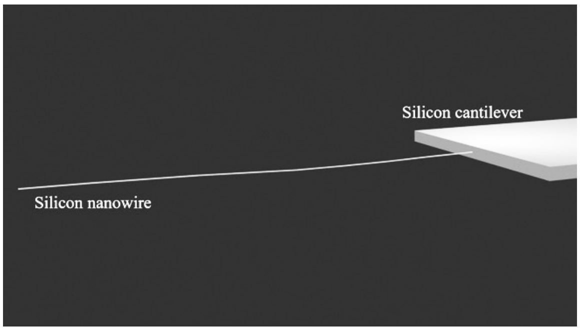

Figure 1: Schematic of a coupled nanowire-cantilever sensor. A high aspect ratio silicon nanowire is attached to the free end of a tipless silicon scanning probe microscopy cantilever.

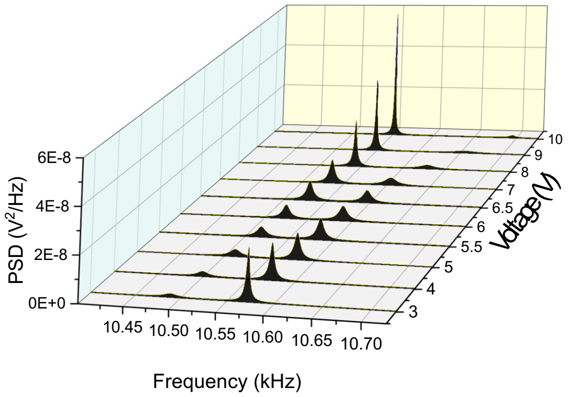

Figure 2: Measured eigenmodes of the co-resonantly coupled system illustrating the effect of electrostatic bias potential application. An avoided level crossing is evident.

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Iron Oxide Nanoparticles as Versatile Nanoscale Reference Materials

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Abstract:

In order to utilize and rationally design nanomaterials, the reliable characterization of their physico-chemical properties is highly important, especially with respect to the assessment of their environmental, biological, and toxicologic impact.[1] Furthermore, regulatory requirements for the registration of nanomaterials, implemented for instance in the REACH Annexes by the European Commission, create a need for the accurate measurement of particle size distributions by manufacturers or analytical facilities. Nanoscale reference materials (nanoRMs) are essential to validate and standardize the methods used to characterize nanoparticle key properties like size distribution, shape, or surface chemistry. However, their availability is limited to very few materials such as polymer, silica, or Au with mainly ideal spherical shapes. Therefore, BAM is currently building up a platform of novel nanoRMs based on iron oxide to provide industrially relevant nanomaterials in various sizes, shapes, and with different surface chemistries.

As a first step, the standard thermal decomposition methods for the synthesis of monodisperse iron oxide nanoparticles[2, 3] were optimized to enable the precise tuning of particle size and shape. Then, reproducibility and scalability were investigated to guarantee the long-term availability of such particles in sufficient amounts and constant high quality. All nanoparticles synthesized by these procedures are capped by long-chain fatty acids that provide excellent colloidal stability in nonpolar solvents. However, some characterization methods require aqueous nanoparticle dispersions. For this reason and for the potential use as test materials in toxicologic or environmental release studies, protocols were established to exchange the hydrophobic surface ligands for hydrophilic citrate or dimercaptosuccinic acid. Furthermore, coating of the iron oxide particles with silica shells of different thicknesses completes this series of potential iron oxide nanoRMs.

As first nanomaterial for certification, we chose cubic iron oxide nanoparticles dispersed in toluene with a nominal edge length of 8 nm . Selected size and shape descriptors, traceable to the SI unit of length, will be certified by transmission electron microscopy (TEM) and small-angle X-ray scattering (SAXS). The particle dimensions determined by TEM as a technique measuring the size of single particles and SAXS as an ensemble method based on a completely different physical principle are in excellent agreement, which makes theses nanoparticles a first valuable reference material for the validation of nanoparticle sizing methods. The stability and homogeneity of the bottled units were ensured for both methods following ISO Guide 35 and ISO 17034. In addition, informative values will be supplied for particle size by dynamic light scattering (DLS) and iron concentration by inductively coupled plasma optical emission spectrometry (ICP-OES).

Keywords: reference materials, iron oxide nanoparticles, electron microscopy, small-angle X-ray scattering, traceability, homogeneity, stability.

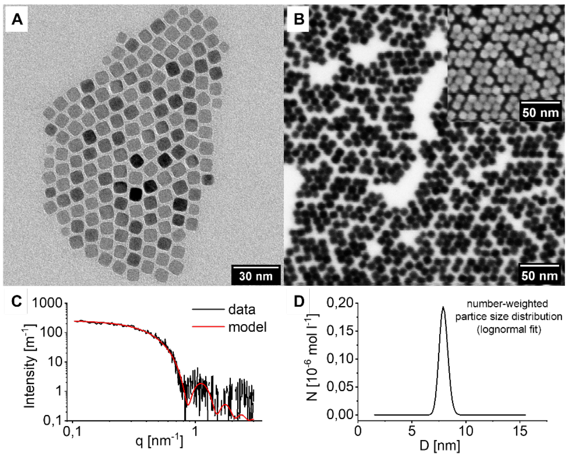

Figure 1: 8 nm iron oxide nanocubes as first nanoRM candidate under certification: representative TEM micrograph (A), STEM-in-SEM micrograph (B, SEM inlens on top-right), SAXS scattering curve (C) and its derived number-weighted particle size distribution (D).

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Tiered Approach Strategy for Occupational Risk Assessment and Management of Lightweight Metals Reinforced with Nanomaterials using Direct Energy Deposition Process

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Abstract:
Nanomaterials (NMs) have been applied in a wide number of industries due to enhanced material properties at the nano-scale. Nevertheless NMs pose several risks to human health, as they have the capability of crossing biological barriers without losing their integrity and reaching some parts of human body inaccessible to larger materials [1]. These risks depend on NMs hazards and exposure potential. As the heath effects associated with the use of NMs are not yet clearly understood, and scarce data exists concerning occupational exposure and occupational exposure limits (OELs), it is necessary to use practices that decrease the risks by encapsulating the NM in a less hazardous material [2] or mitigate the exposure by using gloveboxes and enclosing the process [1].

The NMs occupational risk assessment through the combination of hazard and exposure data, enables the determination of the appropriate level of control measures for risk management [3]. While hazards assessment is based on the characteristics of the materials (toxicology or health effects~~,~~ and physicochemical properties [3]); exposure assessment of workers to NMs requires the establishment of exposure scenarios, which are based on the possible sources of NM emissions, the material physical form, and the characteristics of manufacturing process [3]. In fact, exposure to NMs can occur during any stage of materials life cycle, through inhalation which is the main route of entry into the human body, although skin contact and ingestion are also possible routes of entry [1].

The application of a Tiered approach strategy for occupational risk assessment and management of NMs has several benefits since it is a step-by-step flexible strategy easy to implement and cost-effective because the degree of complexity increases with each step [1, 4]. As a consequence, the level of uncertainty decreases with the increase of the number of tiers providing the support for the decision-making process of suitable control measures.

In this study, a Tiered approach strategy was adopted (namely Tiers 1 and 2), to assess and manage potential occupational risks associated with the use of ceramic NMs (TiC) as reinforcement in lightweight metals (Ti-6Al-4V) using the Direct Energy Deposition (DED) process. In Tier 1, a number of Control Banding (CB) tools, such as Stoffenmanager Nano, Nanotool, and NanoSafer, were used for the initial risk assessment after gathering information concerning the materials, manufacturing process, workplace and existing local control measures. Additionally, the benefits and limitations of the CB tools used were analysed showing that Stoffenmanager Nano was the most complete tool for qualitative and semi-quantitative risk assessment in terms of physicochemical properties and material characterization, exposure characterization on process-related and workplace-related information, as well as for characterization of control measures [5]. For Tier 2, an *in-situ* monitorization of the DED pilot line was performed by gathering quantitative data using Testo DiSCmini instrument with a multi-metric approach to measure potential exposure of workers to NMs. The distinction between the potential emission sources related with the DED process and associated tasks, and the background (NMs emission from external sources) was considered. Finally, based on Tiers 1 and 2 analysis, control measures can be recommended for mitigating the occupational risks to NMs. If control measures are recommended, after their implementation, it is advisible to confirm their efficiency by performing another *in-situ* monitorization (Tier 2).

This study aims at contribute to find useful strategies for occupational risk assessment and management of NMs, evidencing that further research is necessary, considering the diversity of NMs and manufacturing processes available, to ultimately overcome the lack of data on OELs.

Keywords: risk management, tiered approach, nanomaterials, lighweight metals, direct energy deposition.

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The monitoring system of nanoaerosols and noise hazards in an industrial facility based on low-cost environmental sensors

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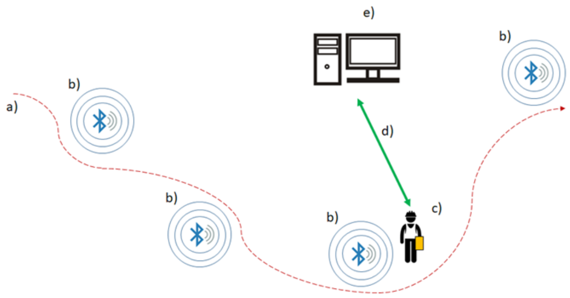
Abstract:

Among the harmful factors related to the work environment, noise poses the greatest threat. The second most frequent harmful factor is dust, including nanoaerosols. An effective solution to this problem may be the continuous monitoring of the parameters of the working environment, enabling the quick detection of areas with high noise emissions and dust concentration and their sources. Due to the dynamic nature of changes and the large terrain, in medium and large enterprises, the use of wireless data transfer seems to be ideal. Thanks to the proposed solution, OSH services will receive a tool for a quick and effective response to exceeded exposure limit values for factors harmful to health, such as noise and dust. Such a solution will also facilitate the assessment of the technical condition of the installation, e.g. detection of leaks, excessive abrasion of elements, faulty operation of mechanical devices.



a) red arrow - employee round route, b) BLE beacons, c) employee during the round, equipped with a portable measuring station, d) green arrow - LoRa wireless connection, e) server and computer with interpreting software data

Figure 1: The basic structure of the dust and acoustic hazard monitoring system.

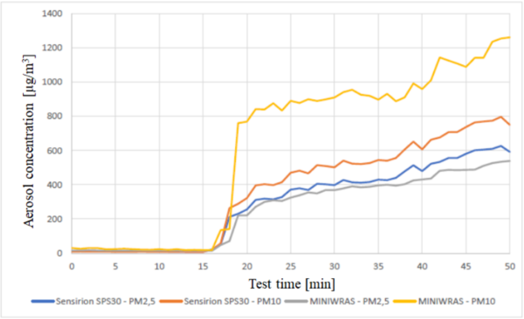


Figure 2: The results of the comparative test of the dust monitoring system with the MiniWRAS spectrometer (dust generator test).

The results of the monitoring system prototype for PM2.5 concentrations of suspended dust are satisfactory. As the MiniWras, the prototype shows high accuracy for the PM2.5 fraction range. The distance between the prototype PM2.5 concentration curve and the spectrometer PM2.5 concentration curve is approximately constant. This means that, assuming the spectrometer as the reference device, the percentage error made by the dust meter in the prototype of the measuring station fluctuates around -2.29% (after calibration). Comparative measurements of A-sound levels for different test signal levels confirmed small differences determined by the developed A-sound level measurement system in relation to the reference meter. Based on the test results, it was found that the prototype can be used as a tool for a quick and effective response to exceeded exposure limit values for factors harmful to health (noise and dust, including nanoaerosols) in an industrial plant.

Keywords: nanoparticles, noise, monitoring system, low-cost sensors, health sciences, environmental engineering

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Acknowledgments

This paper is published and based on the results of a research task carried out within the scope of the fifth stage of the National Programme "Improvement of safety and working conditions" supported within the scope of state services by the Ministry of Family and Social Policy. Task no. 2.SP.15 entitled "Development of a system for monitoring dust and acoustic hazards in close to real time, based on wireless data transmission and portable measuring stations in the work environment". The CIOP-PIB is the Programme's main co-ordinator.

Biotech Session I. A

Laboratory digitalization and automation – the challenges of faster bioprocess development

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Abstract:

Building on the ideas developed more than 10 years ago by Ross King and colleagues [1] among others, one of the great current challenges of modern biotechnological research is the implementation of intelligent solutions in R&D laboratories with the ultimate goal of a robotic scientist. Currently, relatively complex procedures can be carried out in laboratory robots. However, the implementation of intelligent solutions in a closed loop active learning framework is only possible through integrated real-time high-throughput analytics. In other words, also the data must be made available such that they can be used to influence the running experiments, in order to gain maximum information from them, or to directly optimize Key Performance Indicators e.g. maximum product yield according to model bases estimates.

In our KIWI-biolab, we adapt existing Machine Learning approaches to bioprocess optimization by the use of mechanistic models in combination with Machine Learning algorithms (hybrid models). A key to this is the parametrization of mathematical models that describe the complexity of the biological system in the context of the environmental conditions that can occur in a bioreactor. Challenges of the digital twin for biological systems are (i) long lasting historic impacts and the different time constants for the reaction of the different elements of a cellular network and (ii) the close correlation of many parameters and their dynamics over time under the continuously changing conditions in a process. This makes a tight control of the conditions in miniaturized bioreactors very important and challenging. Especially it is important to avoid unfavorable conditions which may not be covered by the model framework [2].

These challenges are also an advantage, because, provided that a biological system can be parametrized with acceptable effort, the digital model can then also be used, for example, for the differentiation and selection of best performing clones (e.g. knockout mutants) [3]. Furthermore, experimental results demonstrate that the parameter sets can describe the cell's phenotype at the appropriate cultivation scale in the context of bioprocess scale up. This is very useful to select already in the phase of early process development clones which are supposed to perform best in the final industrial scale [4].

Keywords: bioprocess development, scale up, fed-batch, machine learning, mechanistic model, Escherichia coli, digitalization, laboratory robot.

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The autotrophic metabolism as interface between renewable energy and redox biocatalysis

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Abstract:

With their excellent selectivity and often very mild reaction conditions, oxidoreductases play an important role in the chemical and pharmaceutical industries. Widely-used enzymatic redox transformations such as C-H oxyfunctionalization or C=C double bond reduction require a stoichiometric supply of electrons, which is usually provided from petrol-based or agricultural cosubstrates such as isopropanol or glucose. The use of an equivalent amount of organic cosubstrates for a process is highly problematic for its atom economy, an important metric for sustainability. This raised a great interest in the utilization of autootrophic microorganisms as means to utilize renewable energy for biotechnological processes.

Whole-cell redox biocatalysis in cyanobacteria uses electrons from photosynthetic water-splitting and would be a radical solution to the problem [1]. Several examples demonstrated the feasibility of the approach with high selectivity and high reaction rates for several redox processes. Similarly, green hydrogen constitutes a clean electron donor for whole-cell biotransformations in hydrogen-oxidizing bacteria [2].

While both strategies would allow significant savings in term of auxiliary cosubstrates and would increase the atom efficiency of redox biocatalysis, the approach needs to overcome several limitations associated to process design and metabolic bottlenecks.

Both strategies would allow significant savings in term of auxiliary cosubstrates and would increase the atom efficiency of redox biocatalysis, but are hampered by bottlenecks associated to the supply of the electron donors and their metabolic utilization. The presentation will discuss approaches how to overcome current limitations in order to improve the volumetric productivity by combining process design and metabolic engineering, and present a strategy towards clean redox biocatalysis in engineered autotrophic microorganisms.

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An enzymatic journey into glycopolymer country

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Abstract:

Glycopolymers, produced by photosynthesis and characterized by an astonishing diversity, are today positioned as very interesting alternatives to synthetic polymers derived from petroleum. The exploration and understanding of their synthesis or functionalization pathway involving enzymes represent a real challenge to access and control new structures.

In this perspective, our work has focused on the understanding of the enzymatic mechanisms involved in the synthesis of microbial α-glucans.

The natural structures that can be obtained from a very simple substrate, sucrose, are surprisingly diverse and depend on the enzymes, glucansucrases and branching sucrases, involved in their synthesis. Structural and functional characterization of a large collection of these enzymes has allowed us to make considerable progress in identifying the structural determinants that control the size, structure and physicochemical properties of these polymers. Based on this knowledge, new polymeric structures and glycoconjugates can be elaborated and designed with engineered enzymes for the development of applications of interest in the pharmaceutical, cosmetic, food, environmental and biomaterials sectors. The oral presentation will provide an overview of the vast potential offered by these approaches.

Keywords: GLycopolymers, polysaccharides, glycoconjugates, enzymatic synthesis, enzyme engineering, biotechnological applications

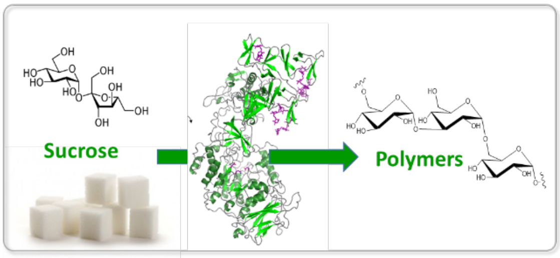

Figure 1: Biosynthesis of a large collections of glycopolymers can be obtained and custom designed by taking adavantage of diversity, structure/function studies and engineering of polymerases and branching enzymes catalyzing sucrose biotransformation.

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Process engineering strategies towards efficient biocatalytic processes

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[2] Institute of Technical Chemistry, Leibniz University Hannover, Germany

Abstract:
The application of nature's catalysts "enzymes" for the synthesis of chemicals is a key emerging field of industrial biotechnology to meet current and future needs of our society for sustainable manufacturing of chemicals. Nature uses an elegant and efficient synthetic strategy: Coupling enzymes in multi-step pathways without intermediate isolation and purification steps with a precise spatial control of catalysis. Inspired by nature, the design of multi-step biotransformations has been attracting great attention within the biocatalysis community.

The keynote talk covers enzymatic (cascade) reactions and demonstration of those at the industrially relevant conditions with the help of process engineering. In particular, two use cases will be introduced covering peroxygenases and decarboxylases in cascading systems exploring the use of non-conventional media and different operational mode for enhancing the efficiency of these enzymatic applications.

Photobiocatalytic Oxyfunctionalization with High Reaction Rate using a Baeyer-Villiger Monooxygenase from *Burkholderia xenovorans* in Metabolically Engineered Cyanobacteria

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[2] Aix Marseille Univ, CNRS, Centrale Marseille, Marseille, France
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[4] Génomique métabolique, Genoscope, Univ Evry, France
[5] Department of Biochemistry, University of Turku, Turku, Finland

Abstract:
The synthesis of ε-caprolactone, an important polymer precursor is currently performed using hazardous peracids from the oxygenation of cyclohexanone[1]. Baeyer-Villiger Monooxygenases (BVMO's), on the other hand could catalyse the same reaction under environmentally-benign conditions[2]. However, the requirement for auxiliary substrates needed for co-factor recycling as well as supplying the necessary oxygen for the reaction hinder this enzymatic route[3]. The recombinant production of BVMO in cyanobacteria allows substitution of auxiliary compounds with water and utilizes oxygen directly from water splitting. Herein, we report the identification of a BVMO from *Burkholderia xenovorans* ($\text{BVMO}_{\textit{Xeno}}$) exhibiting higher reaction rates than previously tested BVMOs in the synthesis of ε-caprolactone. We report a 10-fold increase in specific activity (25 vs 2.3 U g_{DCW}^{-1}) as compared to cyclohexanone monooxygenase from *Acinetobacter* sp. ($\text{CHMO}_{\textit{Acineto}}$). The faster reaction rate and minimal ketoreduction could be attributed to a 10-fold lower K_M value of $\text{BVMO}_{\textit{Xeno}}$ as compared to $\text{CHMO}_{\textit{Acineto}}$. Furthermore, the specific activity was enhanced by further manipulation of the photosynthetic electron transport chain (PETC). The photosynthetic oxygen evolution can contribute to alleviate the highly problematic oxygen mass-transfer limitation of oxygen-dependent enzymatic processes.

Keywords: enzyme catalysis, photosynthesis, Baeyer-Villiger oxidation, biocatalysis, cyanobacteria

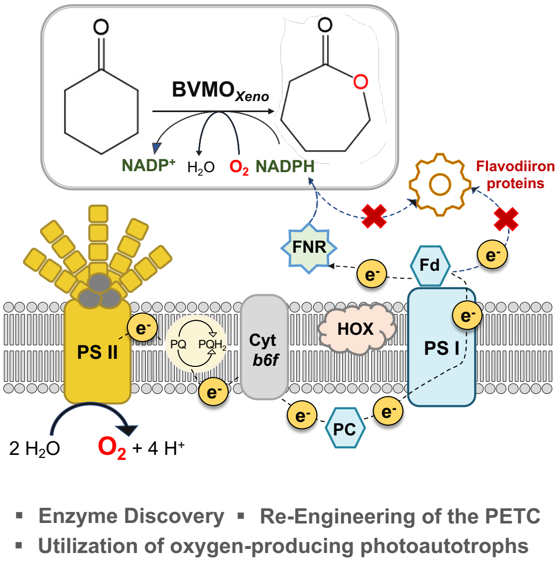

Figure 1: Enzymatic production of ε-caprolactone in metabolically-engineered cyanobacteria.

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Biocatalytic synthesis of novel polyesteramide nanoparticles derived from ε-caprolactam and hydroxy acids

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Abstract:

During the last years, an extensive amount of research has been exploring new possible replacements for non-renewable resources exploited as raw materials by most advanced technologies in the production of polymeric commodities. The development of new biodegradable polymeric materials is currently of great importance considering the environmental hurdle of polymers from fossil raw materials. In this light, an important class of polymers that has recently become more prominent is represented by polyesteramides, as they exhibit enhanced properties on account of integrating both ester and amide bonds in their structure. Polyesteramides are cohering the biodegradability and biocompatibility of polyesters conjoined with the improved thermal and mechanical properties of polyamides, leading to the prospects of valuable applications assigned to their biocompatibility, notably in the biomedical domain, as support matrices for drugs. In other respects, polyesteramides are henceforth foreshadowed to play a growing role as high-performance materials. In the context of polyesteramides synthesis, two key aspects are prevailing, namely employing bio-based raw materials as monomers and the possibility of replacing the classical high-energy-demanding chemical catalysis that can trace toxicity with biocatalysis as an ecofriendly and energetically cost-effective solution. Biocatalytic processes are gaining greater acceptance as they address the need for sustainability. In this work, the biocatalytic approach was assessed for the synthesis of novel polyesteramides derived from ε-caprolactam and different hydroxy acids. The syntheses were carried out in solvent-free systems or in organic solvent for 24 h, at 1200 rpm and temperatures up to 80 °C. Further, the study looked into the synthetic performance of several biocatalysts, including the commercially available immobilized lipases B from *Candida antarctica*, Novozyme 435 and GF-CalB-IM, but also lipase TL from *Pseudomonas stutzeri* and lipase B from *Candida antarctica* immobilized by targeted sol-gel entrapment in our laboratory (Figure 1).

The chemical structures and characteristics of the cyclic and linear oligomeric products were assessed by FT-IR, MALDI-TOF MS, GPC, and NMR analysis. Subsequently, drug-loaded polymeric nanoparticles were prepared from the synthetized polyesteramides using the emulsion-solvent evaporation method, for possible biomedical applications.

Keywords: biobased monomers, enzymatic polymerization, polyesteramides, ε-caprolactam, hydroxy acids, lipase, biomedical applications.

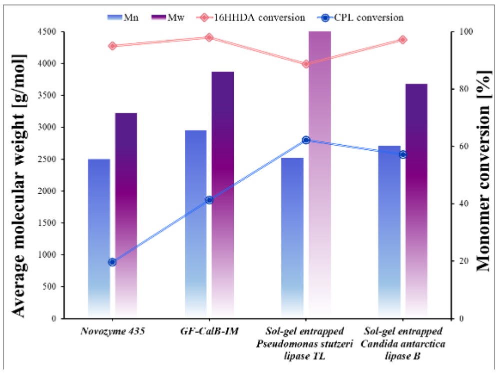

Figure 1: Evaluation of different biocatalysts for the synthesis of ε-caprolactam (CPL) and 16-hydroxyhexadecanoic acid (16HHDA) copolymers.

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Seed Oilcakes Biorefinery as a Promising Renewable Resources for Producing Value-Added Products

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Abstract:

One of the most crucial problems that the world is facing these days is disposing of the petroleum-based plastics since they are not biodegradable and only less than 10% of them are recycled. Petroleum-based plastic application has increased enormously in the last years causing huge waste-disposal problems and a consequent environmental pollution such as releasing of small and toxic petro-polymers in oceans and on the lands swallowed by fish and birds[1]. In order to replace at least a portion of non-biodegradable materials that are currently used in the world and overcome the mentioned environmental pollution the conventional plastics should be replaced with biobased and biodegradable materials.

Soybean (*Glycine max*), is considered as a most cultivated oilseed crop worldwide followed by rapeseed (*Brassica napus*), cotton (*Gossypium hirsutum* L.), sunflower (*Helianthus annuus*), and groundnut (*Arachis hypogaea*). It is worth to say that yearly a huge amounts of waste (almost 600 million tons in 2018/2019, according to USDA) [2] are produced by oil industries and only a small amount of them are utilized as an animal feed, human nutrition, food additives and plant fertilizers, even though most of them are a rich sources of bio-active molecules, fibres, proteins and polysaccharides [3].

The oil industry by-products which known as seed oilcakes (SOCs) can be a potential renewable sources to replace the fossil sources of the plastic materials since they are biobased and biodegradable natural polymers.In this regards, the proteins existing in the SOCs can be considered as an abundant, biodegradable and inexpensive resources for developing edible and environmental-friendly plastics [4].

Keywords: Seed oilcakes, proteins, bioplastics, food packaging, environmental pollution, biorefinery

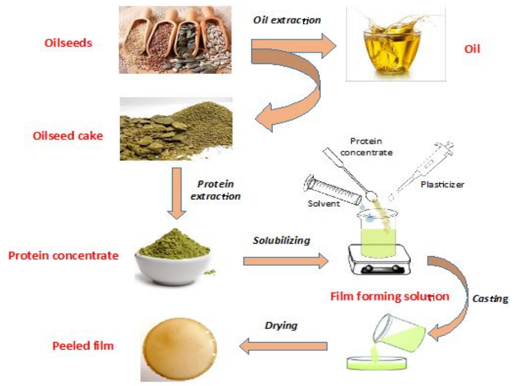

Figure 1: Figure depicting one of the possibilities of seed oilcake biorefining in to the biodegradable protein-based films that can be utilized in several sectors such as food packaging and pharmaceutical. Therefore, among the biopolymers derived from renewable resources, seed oilcakes extracted proteins, without or after purification, could be a potential raw material for bioplastic products since they are abundant, biodegradable and inexpensive.

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Green seaweed – *Enteromorpha* sp. as a feedstock for bioprocess engineering

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Abstract:
Green seaweeds constitute a valuable feedstock, rich in bioactive compounds. However, in many countries, this biomass is treated as waste. In the present study, we propose many approaches for seaweeds bioprocessing into valuable bioproducts (Figure 1). As dry biomass, it can be directly used as a biosorbent to remove heavy metal ions from wastewater or to bioremediate soil contaminated with metal ions by their immobilization. The application of innovative extraction techniques, such as ultrasound-assisted extraction or enzyme-assisted extraction enables the conversion of algal biomass into products useful for agriculture, for example, biostimulants of plant growth. Seaweed extracts can also be used for the biosynthesis of metal nanoparticles, with multifunctional properties and applications (for example agriculture, environment protection, medicine, etc.). In the present work, we focused mainly on the production of biochar from green macroalga *Enteromorpha* sp. by pyrolysis at temperatures 300, 500, and 700°C. This biochar was characterized in terms of multi-elemental composition, BET surface area, total pore volume, as well as biosorption properties towards phosphorus ions. The highest surface area was obtained for biochar produced at 700°C – 25 m^2/g. In order to increase the sorption capacity of biochar, it was modified with $MgCl_2$. Modified biochar produced at 700°C was able to remove 84.3% of the phosphorus from the wastewater, whereas non-modified only 40.6%. Biochar enriched with phosphorus can serve as a valuable soil amendment. The pot experiments performed on winter wheat (*Triticum aestivum*) with the 3% addition of dry *Enteromorpha* sp., pristine biochar, and Mg-modified biochar enriched with phosphorus showed that these amendments stimulated plant growth (length and weight of plants) as well as the chlorophyll content in leaves. Our results indicate that the production of biochar (pristine and Mg-impregnated) is a sustainable option to valorize the biomass of seaweeds, as well as to recycle phosphorus from wastewater.

Keywords: green seaweeds, biosorbents, biosorption of metal ions, wastewater treatment, bioremediation, heavy metal polluted soil, innovative extraction techniques, seaweed extracts, biostimulants of plant growth, biosynthesis of metal oxide nanoparticles, pyrolysis, biochar, soil amendment

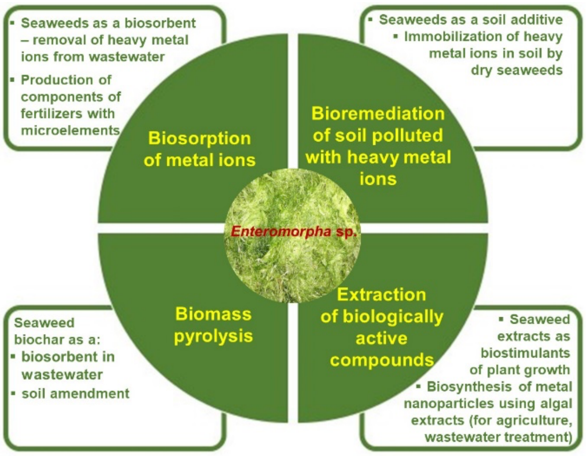

Figure 1: Multitude applications of *Enteromorpha* sp. biomass.

Acknowledgments
This work was performed in the framework of grants: “Eco-friendly technologies for the management of seaweed biomass for products useful for sustainable agriculture and biosorbents used for the removal of heavy metal ions from the environment” (2019/33/B/NZ9/01844) from the National Science Centre in Poland and “Valorization of the waste macroalgae biomass into bioproducts useful for sustainable agriculture and environment” from the Polish National Agency for Academic Exchange (NAWA-Canaletto, PPN/BIT/2021/1/00004/U/00001).

Engineering Methyltransferase Pathways for Selective Chemical Tracking of Epigenetic Writers in Mammalian Cells

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Abstract:

Enzymatic methylation of cytosine to 5-methylcytosine in DNA is a fundamental epigenetic mechanism involved in mammalian development and disease. DNA methylation is brought about by collective action of three independently expressed and regulated AdoMet-dependent proteins (Dnmt1, Dnmt3A and Dnmt3B). Loss of Dnmt1 is directly linked to tumorigenesis and chromosomal instability, whereas Dnmt3b mutations cause a severe autosomal disease, called ICF syndrome. However, the catalytic interactions and temporal interplay of these epigenetic "writers" in establishing and maintaining genomic DNA methylation profiles characteristic to each cell type are poorly understood. To dissect the catalytic action of an individual Dnmt enzyme, we used structure-guided engineering of the mouse Dnmt1 (residues 291–1620) for the transfer of bioorthogonal 6-carbon linear moieties containing a functional azide group onto DNA from a synthetic cofactor analog, Ado-6-N_3 *in vitro*. Examination of the produced Dnmt1 mutant pool in vitro yielded a variant that conferred a 8400-fold improvement in cofactor selectivity as compared to the WT enzyme. To establish endogenous expression of the cofactor-engineered version of the enzyme in mouse embryonic stem cells, we installed the corresponding codons in the Dnmt1 alleles using CRISPR-Cas9 genome editing. Further, we found that pulse-internalization of the Ado-6-N_3 cofactor by electroporation into the engineered cells enabled selective catalysis-dependent azide-tagging of Dnmt1-specific targets *in vivo*. The deposited chemical groups were exploited as 'click' handles for reading adjoining sequences and precise mapping of the tagged methylation sites in the genome using TOP-seq. Altogether, we demonstrate the first general approach that produces high-resolution genome-wide temporal "tracks" of the Dnmt1 catalysis in live mammalian cells during the cell cycle or differentiation to somatic lineages, offering unprecedented inroads into studies of genomic methylation in a wide range of eukaryotic model systems.

Keywords: DNA methylation, pathway engineering, chemical tagging, AdoMet cofactor analogs, epigenome profiling, cell technology.

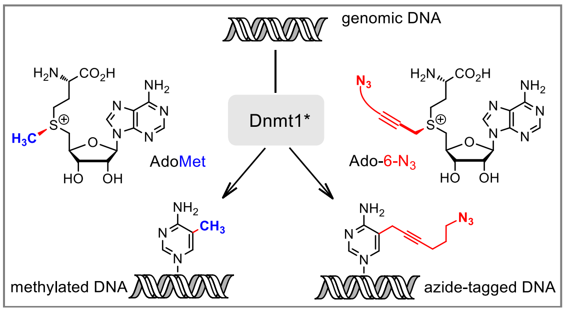

Figure 1: Strategy for catalytic activity-based azide-tagging of Dnmt1 target sites using an engineered (Dnmt1*) enzyme and pulse-delivered synthetic Ado-6-N3 cofactor analog in live mammalian cells.

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Evolution-guided metabolic engineering for improving synthetic, genome-reduced co-cultures of *C. glutamicum*

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Abstract:
We successfully created synthetic communities of niche-optimized strains (CoNoS) [1] that consists of two strains of the same species *Corynebacterium glutamicum* that are mutually dependent on one amino acid [2]. We used both the wild-type and the genome-reduced C1* chassis [3] for introducing selected amino acid auxotrophies, each based on complete deletion of all required biosynthetic genes.

By sharing enzymatic capacity for amino acid synthesis, CoNoS offers a valuable approach for redirecting carbon and energy sources toward higher microbial production of small molecules. However, establishing stable and fast-growing CoNoS requires optimization of cross-feeding interactions, which can be challenging. To improve the growth of our CoNoS designs, we combined two approaches.

A first round of rational metabolic engineering based on known targets resulted in enhanced amino acid exchange between community members and stable co-culture growth. With this premise, we then performed automated adaptive laboratory evolution experiments on a Mini Pilot Plant [4] to induce mutations that were beneficial to the synthetic community (Figure 1). Genome sequencing of the isolated mutants revealed new targets and provided deeper insight into amino acid metabolism in *C. glutamicum*. Specific targets for improved amino acid exchange were used to further reverse engineer selected CoNoS, leading to successful optimization of growth and amino acid production performance of our synthetic co-cultures.

Keywords: microbial communities, synthetic co-cultures, *C. glutamicum*, genome reduction, adaptive laboratory evolution, amino acid production

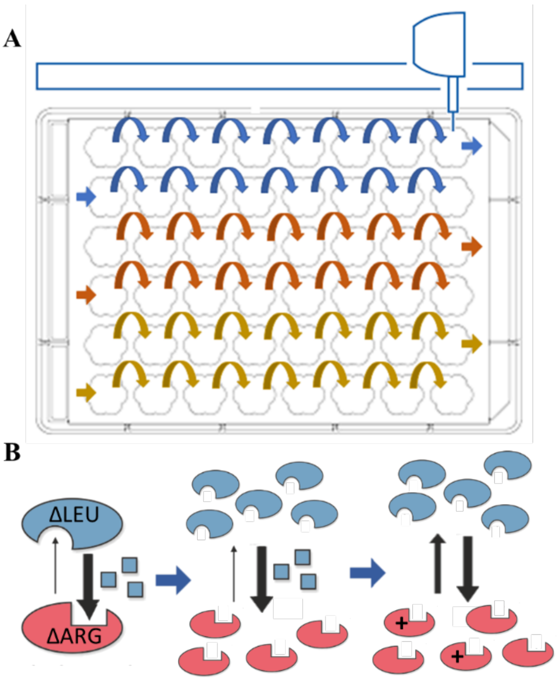

Figure 1: Schematic representation of automated repetitive batch cultivation in microtiter plates (A) triggering the evolution-guided metabolic engineering of CoNoS (B) to solve the bottleneck of limited amino acid exchange.

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What if *Escherichia coli* fails? Exploiting an Antarctic bacterium for the production of proteins harbouring intrinsically disordered regions

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Abstract:
Eukaryotic protein kinases regulate most biological processes. However, the study of such proteins is sometimes limited by the unavailability of suitable protocols for their recombinant production and purification. One reason behind this difficulty can be traced to the structural features that they share. Many regulatory proteins indeed are hybrid proteins containing both a structured catalytic domain and intrinsically disordered regions (IDRs), mainly involved in the interaction processes with their substrates[1]. This is the case of *h*CDKL5, a hybrid human kinase difficult to obtain from recombinant sources. Its expression in *Escherichia coli* indeed results in totally insoluble and inactive products[2]. In this work, we demonstrated that the Antarctic bacterium *Pseudoalteromonas haloplanktis* TAC125 (*Ph*TAC125) can produce *h*CDKL5 as a soluble active form, introducing it as an alternative cell factory for the production of "difficult" proteins (Figure 1). To achieve such a result, novel recombinant production systems were established and implemented in the psychrophilic bacterium. First, we combined the development of an IPTG-inducible plasmid with *Ph*TAC125 strain engineering aimed at enhancing the recombinant expression and inducer uptake[3]. Then, we focused on the expression vectors. The origin of replication was mutagenized so to obtain high copy number vectors, while the cassette of expression was arranged in a bicistronic asset to enhance the translation efficiency of unstable transcripts. This multiparameter approach led to a recombinant production yield of 5 mg of protein per litre culture. The catalytic activity of *h*CDKL5 purified from *Ph*TAC125 was confirmed via in vitro kinase assay. In addition, we further implemented the bacterial system for in vivo activity studies. The development of a plasmid harbouring a tricistronic design allowed for co-expression of the kinase with its natural substrate, EB2[4]. The measurement of the phosphorylation occurring in vivo on EB2 was directly correlated to the activity of the human kinase, paving the way for the exploitation of this platform to study the biology of hCDKL5.

The overall efforts succeeded in the construction of an unconventional cell factory exploitable for both the expression of hybrid unstructured/structure proteins and as a model system for studying their functions and pathological alterations.

Keywords: *Pseudoalteromonas haloplanktis* TAC125, cell factory, strain engineering, recombinant protein production, intrinsically disordered proteins.

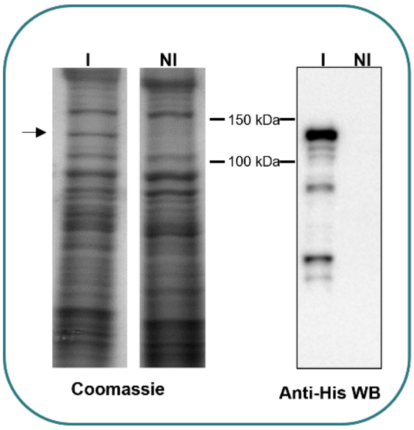

Figure 1: Production levels of *h*CDKL5 in *Ph*TAC125. Total lysates of induced and non-induced cultures were analyzed via Coomassie staining (left panel) and Western blotting (WB, right panel). The overexpression band detected after Coomassie staining is highlighted by a black arrow.

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Membrane transporter identification and modulation via adaptive laboratory evolution

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Abstract:

Membrane transport proteins are potential targets for medical and biotechnological applications. However, more than 30% of reported membrane transporter families are either poorly characterized or lack adequate functional annotation. Here, adaptive laboratory evolution (ALE) was leveraged to identify membrane transporters for a set of molecules as well as specific mutations that modulate the activities of these transporters. In the first case study, a naïve *E. coli* strain was adaptively evolved under increasing concentrations of four amino acids separately in parallel evolution experiments. Resequencing of the evolved strains revealed a diversity of mutations across all evolved lineages, which modulates the activities of specific membrane transport genes. The causality of these mutations were assessed and the activities of the affected transport systems were evaluated through a series of demonstrations including transcriptomics and fluorescence based transport assays. Additionally, a small scale fermentation experiments exemplified the role of transporter overexpression on the production rate of an amino acid. In another case study, the ALE approach applied for a systematic discovery of redundant Multidrug Transporters (MDTs) in bacteria. To that end, a naïve *E. coli* strain and its cognate major MDTs knockouts were evolved separately under higher concentrations of two lipophellic cations. Resequencing of the evolved mutants revealed a backup compensation transporters with overlapping functionality that cover the loss of the deleted MDTs. The detailed regulatory and coding mutations observed in the discovered MDTs pinpointed the effeciency of ALE to explore the versatility of the bacterial transporter ensemble. The broad applicability of ALE to a range of microbes[1] holds great promise for the identification of transporters for a range of molecules and microbes of interest. Subsequently, ALE can be scaled as a systematic and efficient approach to drive basic discovery efforts of membrane transporters that have medical and biotechnological relevance.

Keywords: membrane transporters, adaptive laboratory evolution, *Escherichia coli*, Multidrug Transporters, amino acids, lipophellic cations

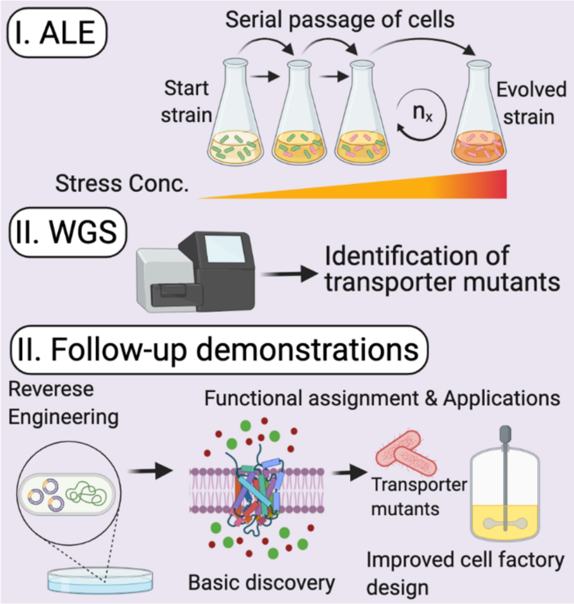

Figure 1: The ALE workflow, coupled with whole genome resequencing, as a method to assign a functional role to individual transporter proteins without requiring *a priori* knowledge. Discovered transporter mutants could be utilized to drive basic discovery efforts of membrane transporter mechanisms that have medical and biotechnological relevance.

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Engineering *Escherichia coli* to produce industrially relevant oleochemicals

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Abstract:
The global demand for oleochemicals, such as fatty acids, is steadily increasing. These compounds cover a large variety of industrial applications ranging from cosmetics over bioplastics to biofuels. However, certain oleochemicals, like unsaturated medium chain fatty acids, currently come with a high production cost which heavily hinders industrial applications. Recent advances in metabolic and genetic engineering have put forward bacteria as promising production factories for these compounds. However, enzymes and cell factories need to be optimized to reach industrially applicable production rates. The aim of the current project was to increase the production of industrially relevant oleochemicals in the model organism *E. coli.*

E. coli naturally produces only a limited range of oleochemicals. To unlock the production of diverse, industrially relevant oleochemicals, exogenous enzymes from various sources were codon optimized and introduced. Expressing those enzymes led to a shift of the carbon flux towards desired oleochemicals. To illustrate, when desaturases from plants were expressed, the level of unsaturated fatty acids increased significantly.

This basal production of oleochemicals was then further increased by deactivating competitive pathways or reactions. Appropriate candidates were identified using constraint-based metabolic flux modelling. In detail, a genome-scale metabolic network model from *E. coli* was adapted to included and furtheron used with the OptKnock algorithm. It calculates which gene deletions would theoretically lead to an increase of the carbon flux towards the desired oleochemical. By constructing the knock-out strains we could indeed validate this computational approach.

By introducing exogenous enzymes and knocking out competitive pathways, we succeeded in designing microbes that show an elevated production of specific oleochemicals. In a next step, In a next step, production conditions were optimized in lab-scale bioreactors.. Ultimately, this will lead to microbes which can be used in bioprocesses and open a hitherto unlocked industrial potential.

Keywords: oleochemicals, microbial production, metabolic simulations, enzyme expression

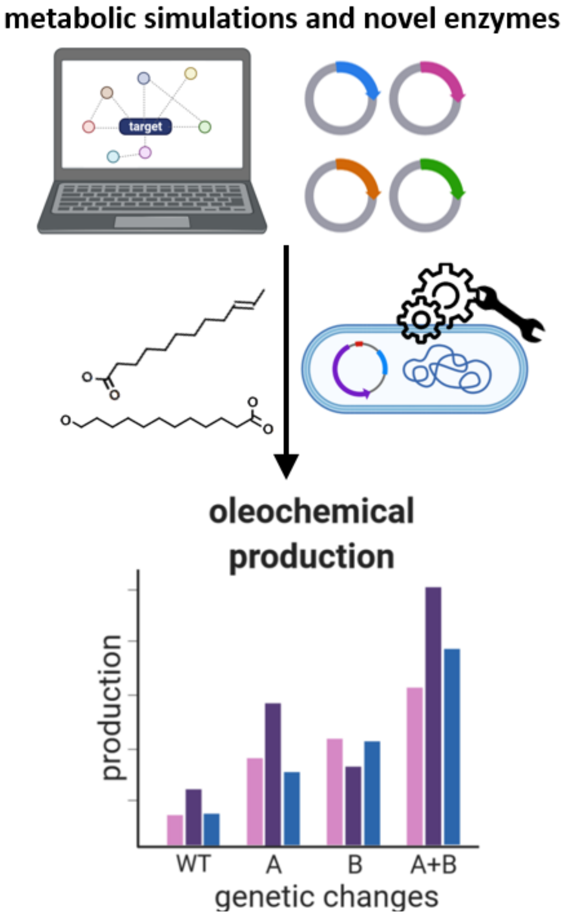

Figure 1: Workflow to produce industrially relevant oleochemicals using *Escherichia coli*. Expression of exogenous enzymes forces the cells to produce various oleochemicals. This production is further increased by deleting competitive pathways, which are identified by metabolic simulations.

Microencapsulation of primary human tonsillar B cells for directed *ex vivo* cultivation platform

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Abstract:
B cells play a vital role in the immune system response against a variety of pathogens encountered throughout life. Understanding the mechanism of B cell proliferation and maturation through cytokines interaction and additional stimulation has been a research focus of the past decades. *Ex vivo* cultivation methods of B cells mostly rely on suspension cultures which are incapable of emulating the complex nature of secondary lymphoid organ tissues. Microencapsulation provides the opportunity to more closely mimic *in vivo* environments in which B cells grow and mature, allowing for more realistic *in vitro* cultivation conditions. By encapsulating B cells, higher local cell densities can be realized in a biomimetic microenvironment, which can be self-conditioned by the encapsulated cells through potentially enhanced autocrine factor accumulation and improved cell-to-cell contacts. Based on previous work on the encapsulation and cultivation of T cells, we propose an encapsulation method utilizing sodium cellulose sulfate (SCS)/poly(diallyldimethyl) ammonium chloride (PDADMAC) capsules, with the ability to direct B cell proliferation and differentiation through the co-encapsulation of important signaling molecules.

Primary human tonsillar B cells were isolated and cultivated in a suspension culture system for cell expansion and differentiation based on CD40L stimulation. A microencapsulation unit was developed and 3D-printed in-house for production of SCS/PDADMAC microcapsules, resulting in uniform spherical capsules with a diameter of 1223 ± 47 µm. Diffusion experiments showed that molecules bigger than 10 kDa were held back inside capsules, meaning that signaling molecules for B cell expansion and differentiation larger than 10 kDa (CD40L, IL-4, IL-21, BAFF) could be incorporated inside capsules. Encapsulated cell growth and differentiation were monitored through live/dead and immunostaining, respectively.

Encapsulating B cells reduced overall cell expansion compared to parallel control suspension cultures. Increasing the amount of CD40L-per-cell inside capsules to reach the level used in non-encapsulated cells cultivation improved cell proliferation. Thus, growth rates similar to suspension cultures could be achieved. In suspension cultures, memory B cell phenotype differentiated towards plasmablasts, while performing a plasma cell (PC) burst, peaking after 4 – 6 days of culture. Encapsulation of B cells strongly altered this differentiation behavior. Rather than a burst, PC content increased steadily over time, indicating the development of more long-lived PC. Most notably, the development of germinal center phenotype was observed in encapsulated cultures, whereas no such development was present in suspension cultures. Overall, B cell microencapsulation led to a broadened differentiation potential of encapsulated cells, showing its potential as a platform for enhanced *ex vivo* B cell cultivation and maturation. Encapsulation of B cells is a promising approach as a basis for *ex vivo* immunization therapies or the production of polyclonal antibodies.

Keywords: *ex vivo* B cell cultivation, microencapsulation, biomimetic microenvironment, soluble CD40L stimulation, germinal center cell development

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Multifaceted Roles of Versatile LEA-II Proteins from Cereals and Date Palm

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Abstract:

Late Embryogenesis Abundant (LEAII) proteins are mostly predicted to be intrinsically disordered proteins (IDPs) that are induced under conditions of cellular dehydration. LEA-II proteins play a vital role in plant's responses to abiotic stresses. They are also claimed to stabilize macromolecules against damage caused by heat, freezing, dehydration, ionic or osmotic stresses. In date palm, LEAII genes are highly abundant (Figure1). Their functions, however, are largely unexplored and also their structure and interactions with potential target molecules have only recently been investigated in a small number of proteins. We report the overexpression of DHN-5 from wheat, a distinct biochemical group of LEAII proteins, in Arabidopsis generates enhanced tolerance to salt and osmotic stress and leads to wide transcriptome changes on abiotic and biotic stress tolerance genes. MDHAR gene (Monodehydroascorbate reductase) involved in the ascorbate biosynthetic pathway was up-regulated and correlated with higher ascorbate content (antioxidant) in transgenic lines. The DHN-5 transgenic Arabidopsis plants are less sensitive to Jasmonate and affects a subset of JA-responsive genes. Our study suggests further functional properties of LEA-II proteins in protecting membranes, stabilizing macromolecules, aiding in free radical scavenging and acting as antioxidants for alleviating the oxidative damages caused to plants under the climatic stress. Moreover, DHN-5 and date palm LEAII proteins improved the thermostability and the enzymatic activities in vitro of β-glucosidase (bglG) and Lactate Dehydrogenase (LDH) at 70°C and 50°C, respectively. The truncated forms of DHN-5 containing only one K- or two K-segments are able to protect the LDH and bglG activities under various stress treatments *in vitro*. Our results indicate that LEAII proteins from wheat and date palm exhibit myriads of functions with potential applications at the industrial level.

Keywords: LEAII proteins, abiotic stresses, enzymatic activity, transcriptome, pleitropic effects, industrial applications.

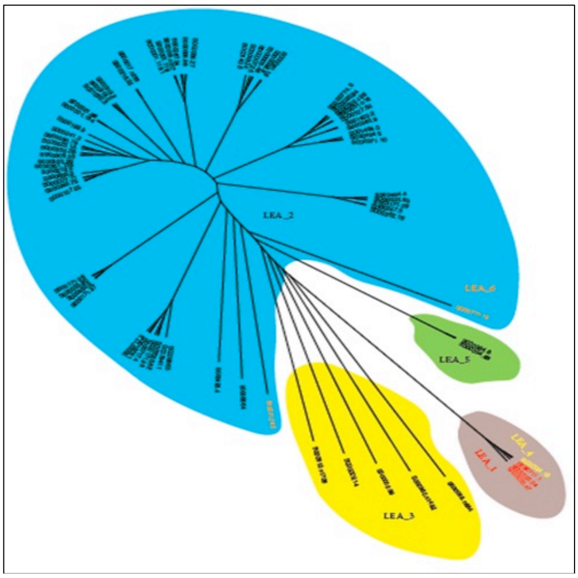

Figure 1: Phylogenetic tree showing the abundance of LEAII genes in date palm.

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The Ethics of synthetic meat. Hypes and hopes of a new challenging technology

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Abstract:
The Ethics of synthetic meat is an emerging field in applied Ethics. As the world's population grows, stakeholders, scholars and manufacturers have begun to hypothesize new strategies to meet growing food needs and to prevent food production from having a deleterious environmental impact. Among the various strategies adopted, the creation of synthetic meat deserves special mention. This technology has aroused both hopes and fears among consumers and scholars involved in the agri-food sector and, lately, among moral philosophers.

In this contribution I will focus on the main moral arguments against the production and consumption of synthetic meat, particularly showing how none of them seems to be particularly convincing.

I will then highlight how important the contribution of philosophy is in structuring good arguments in favor of the diffusion of this kind of technology and for the very growth of consumer trust.

However, I will also underline how sometimes expectations for this kind of product encourage an underestimation of the needed structural transformation of the eating styles of Western countries and the need to invest in organic plans to satisfy the food requests of developing countries. Ultimately, it will be suggested to adopt a multifocal approach that is also able to include the production of synthetic meat, as a product that can partially alleviate the environmental impact of meat production and partially prevent animal suffering. Not investing in this new possibility offered by biotechnological developments prevents us from benefiting from a useful tool that could enhance our living condition.

Keywords: cultured meat, non-human animals, animal welfare, environement, ecological impact, multifocal strategies

Figure 1. Synthetic meat (also known as cultured meat or clean meat) consists of animal cells taken by biopsy that undergo a process of differentiation and proliferation in a culture medium. Until recently, this was fetal bovine serum. The use of this medium has raised some concerns among scholars. Currently, companies such as Mosa Meat have overcome this critical issue by identifying valid alternatives

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Nanotech / GAMS / Biotech
Joint session II.

Making the enzymatic synthesis of bio-based polyesters feasible: from bioinformatics to pilot plant

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Abstract:

Biocatalysis offers well established knowledge and tools, such as hydrolases enzymes, for boosting the implementation of bioeconomy and, more specifically, bio-based chemistry. The ability of enzymes to catalyze transformation of solid substrates or solid surfaces represents an added value in terms of environmental and economic sustainability of processes, where the solvent can be minimized or avoided. However, designing and synthetizing novel products endowed with unprecedented properties require a fine integration of reaction engineering with enzyme screening and organic chemistry.

The present communication will discuss the integration of experimental strategies with molecular modeling (Figure 1) and bioinformatics methods based on molecular descriptors. The analysis allowed the understanding of similarities and differences of cutinase and lipase enzymes, two classes of hydrolases that were applied for the solvent-free synthesis of structurally different polyesters, not obtainable through conventional chemical polycondensation. The economic and environmental parameters of the reactions were considered to enable the scaling up of the synthesis, also paying attention to the sustainability of the immobilization process. Different bio-based monomers were employed to obtain oligoesters with controlled architecture and endowed with functional groups prone to further chemical modifications. Results indicate that solvent-free biocatalysis is feasible on larger scale as long as new reactor configurations suitable to overcome viscosity and mass transfer limitations. Moreover, DoE trategies pointed out how the role of the biocatalyst is limited at the first stage of the polycondensation, thus enabling the early recovery and reuse of the enzyme. Inexpensive and sustainable immobilization carriers were also tested for improving the economic viability of the process.

Keywords: Biocatalysis, bio-based polymers, bioinformatics, enzyme immobilization, enzymatic polycondensation.

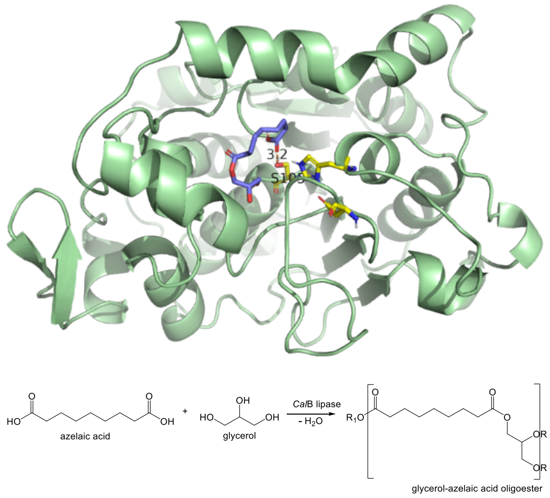

Figure 1: 1-monoacylated glycerol docked in the active site of a lipase for the understanding of regioselectivity of enzymatic polycondensation. The catalytic Ser is in yellow, whereas the substrate is purple.

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Acknowledgement

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Use of a Microbioreactor for Screening of Fungal/Bacterial Co-culture Activity against a *Fusarium* Strain

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Abstract

The Fusarium genus is the cause of several plant diseases that can have a great variety of targets and of consequences for plant crops, their yield and the health of the consumers. Among them, *Fusarium graminearum* and *Fusarium oxysporum* are the most economically impactful. Sustainable means of warfare against these pathogens are currently limited. Biocontrol is an alternative solution to phytochemical pesticides. However, it remains difficult to fully harness the potential that exists in nature. A notable mean of discovering new interactions, in particular between microorganisms is co-culture. The main idea behind this project was to put fungal and bacterial strains together in a liquid medium allowing the growth of both participants. The number of strains and therefore of combinations tested, required the use of microbioreactors at first. Thus, ten different bacterial and fungal strains and twenty-five fungal/bacterial co-cultures were cultivated in two different media conditions, and tested for their activities against a *Fusarium* strain isolated from wood and a yeast strain (*S. cerevisiae*). Most of the co-cultures showed a development of the two partners or a modification of the growth of one of them (Figure 1). Furthermore, several co-cultures also showed an activity against the selected targets. This allowed a first screening of interesting activities and a selection of strains and co-cultures of interest. The criteria for the first choice of the strains and the consequent use of the microbioreactor will be detailed.

Keywords: phytopathogenic fungi, *Fusarium*, antifungal activity, microbioreactor, biocontrol, fungal/bacterial co-culture

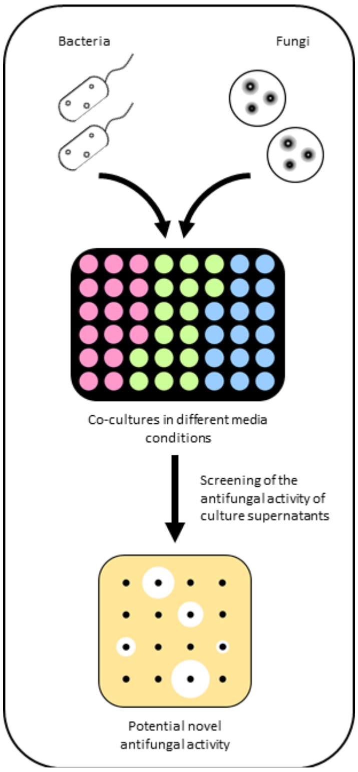

Figure 1: Figure illustrating the idea behind the project of co-cultivating bacteria and fungi strains in a microbioreactor to screen them for their antifungal activity and eventually discover novel activities.

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Stereoselective synthesis of whisky lactones catalysed by bacteria from *Rhodococcus erythropolis* species

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Abstract:

Lactones are aroma compounds that are widely used in industry as a fragrance ingredients in various foods such as sweets, drinks, baked goods. Among them whisky lactone is an essential component of aged alcoholic beverages such as whisky, cognac, and brandy beverages. *Cis* whisky lactone-isomers are described as earthy and woody fragrances, while *trans*-isomers are reminiscent of celery. Whisky lactone is not only an aroma; the mixture of *cis*-and *trans*-isomers is used as a repellent against mosquitoes and flies.

There are several stereoselective pathways for the synthesis of *trans*- and *cis*- whisky lactone isomers, however they rely on multistep chemical synthesis using metal catalysts and organic solvents. Therefore, it is important to develop biological methods such as biotransformations to obtain individual lactone isomers [1].

Biotransformation is a process in which microorganisms or isolated enzymes are applied to obtain fine chemicals, such as enantiopure forms of chiral compounds. Obtaining the desired products by the use of environmentally safe biocatalysts and raw materials makes this approach possible to meet the requirements of sustainable development and green chemistry [2].

Series of experiments were carried out to compare the biotransformation carried out in Submerged Fermentation (SmF) with those conducted in Solid State Fermentation (SSF). A synthetic medium was used for the biotransformation in SmF, while agro-industrial side streams such as linseed, rapeseed and primrose cakes were used for SSF.

In preliminary screening transformations, based on significant oxidation activity a wide range of whole bacterial cells were tested. Among tested bacteria, the transformation carried out with *Rhodococcus erythropolis* led to the formation of whisky lactone isomers with the highest enantiomeric excesses. Significant differences in the course of the process in SmF and SSF were observed. In SmF conditions enantiomerically pure *trans*-(+)- (4*S*, 5*R*), *trans*-(-)-(4*R*, 5*S*) and *cis*-(+)-(4*R*, 5*R*) isomers were obtained, while in biotransformations conducted in SSF only enantiomerically enriched *trans*-(+)-(4*S*, 5*R*), *cis*-(+)-(4*R*, 5*R*) and *cis*-(-)-(4*S*, 5*S*) isomers were obtained [3].

Keywords: biotransformation, microbial oxidation, whisky lactones, diols, submerged fermentation, solid state fermentation.

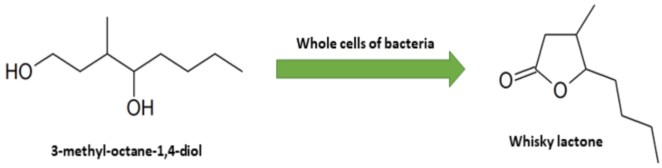

Figure 1: Figure illustrating scheme of the presented biotransformation.

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Fungistatic potential of *Apiaceae* lactones and their derivatives

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Abstract:
Microbiological food spoilage is the cause of **huge losses in the food industry**, estimated at 25% of the total production, due to its significant quality changes [1].This generates the need for food additives, especially preservatives. Taking into account consumer preferences, extension of food shelf-life using agents of natural origin is a topic of considerable interest [2]. **Compounds with a lactone group** present in plants of the *Apiaceae* family are in line with this trend. Moreover, some of this group of compounds such as 3-*n*-propylidenephthalide, 3-*n*-butylphthalide, 3-*n*-butylidenephthalide have been approved by the European Food Safety Authority in the Commission Implementing Regulation (EU) No 872/2012 for use as food flavourings [3].

The aim of the research was to determine the **fungistatic** activity of seven lactones against *Rhodotorula mucilaginosa* IHEM 18459, carotenoid-producing yeasts causing spoilage of dairy products [4-5]. For this purpose, compounds were tested using **microdilution broth method**. Next, the most effective lactone, 3-*n*-butylidenephthalide (Figure 1), was tested at the **macroscale**. Yeast dry biomass, fatty acid methyl esters (FAME) content and their profile were determined for the cultures with different concentration of the added fungistatic.

It has been observed that **biomass content declined** with rising content of lactone, which proved the inhibiting properties of a compound. An additional effect observed during the study was a change in the color of the *Rhodotorula* cultures, induced by the compound. This prompted the investigation on the **alteration of different carotenoid pigments profile** in the cultures.

Keywords: lactones, bioactivity, fungistatic, antifungal, natural compounds

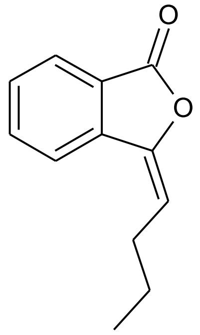

Figure 1: Structure of 3-*n*-butylidenephthalide, natural fungistatic used in the research

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Effect of acid pretreatment on the primary products of biomass fast pyrolysis

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Abstract

A high load of inorganics in raw lignocellulosic biomass are known to inhibit the yield of bio-oil and alter the chemical reactions during fast pyrolysis of biomass. In this study, the effect of water and acid leaching on the inorganic content and on the primary products distribution during fast pyrolysis of palm kernel shell (PKS), mahogany (MAH) sawdust and iroko sawdust was investigated. Fast pyrolysis was carried out at 600°C and 5s with a micro-pyrolyser connected to a Gas Chromatograph-Mass Spectrometer/Flame Ionisation Detector (GC-MS/FID). Compared to the other acids, HCl was the most effective to remove inorganics from the biomass. Acid leaching prior to pyrolysis resulted in increased production of sugars especially levoglucosan. The highest relative content of the sugars was achieved for the biomass pretreated with H_2SO_4 which was due to the increased production of levoglucosenone. Additionally, the formation of furfural (furans) was increased to a large extent, especially for the biomass sample pretreated with H_2SO_4. A general increase in the relative content of the phenols was also observed for the woody biomass (MAH and IRO). However, no major difference was found for PKS while there was a generally decreased in the relative content of the acids and ketones for all three biomass across the different leaching solutions. This study shows that the production of some valuable chemicals could be promoted by pretreatment with different acid solutions.

Keywords: Fast pyrolysis; Primary products; Pretreatment of biomass; Py-GC/MS/FID

Explanatory note

Pyrolysis is a thermal process used for the decomposition of solid lignocellulose biomass to produce bio-oil and valuable chemicals. Fast pyrolysis is a rapid heating process occurring at elevated temperature and short residence time and used mainly for bio-oil production purpose. In this study fast pyrolysis has been used to investigate the effect acid washing on the product distribution of raw and pretreated palm kernel shell, mahogany and iroko sawdust with the use of Py-GC/MS/FID instrument. This instrument uses a platinium filament that can be used to generate fast temperature rise time and precise temperature control when the biomass sample in direct contact with it is heated by a powerful current pulse. The method applied enables the investigation of isothermal primary reactions due to its high heating ramp of about 100000 °C/s, and a chamber temperature of 150°C that minimizes secondary reactions. The product distribution from the experiment were identified with the mass spectrometer and quantified by the flame ionization detector. The volatiles obtained were further confirmed with the NIST library (NIST MS Search 2.0).

Figure 1: Pyrolysis Unit with Platinum Filament

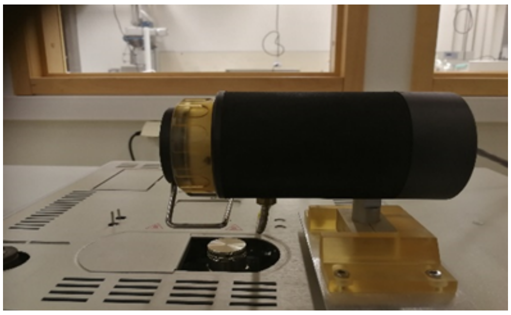

Figure 2: Pyrolysis Unit

Much More than Salts and Mixtures: Functionalized Ionic Liquids and Eutectic Systems for Biomolecules Purification, Greenhouse F-gases Separation, and Drug Formulation

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Abstract:
An emerging research field of interest is the use of ionic liquids (ILs) and eutectic systems (DES) in aqueous biphasic systems (ABS), gases absorption and pharmaceutical applications.

Recently, we proposed a benign route for ABS containing cholinium-based ILs,[1] disclosed novel ABS composed of fluorinated ILs (FILs) [2] and demonstrated that FILs reduce the impact of the addition of water upon the IL's H-bond acceptance ability.[3] Herein, bioprivileged ILs and DESs were implemented to develop more versatile and amenable to be tuned ABS. To understand their potential as extractive platforms of biomolecules, the ternary phase diagrams, the polarity parameters of the coexisting phases, and the partition coefficients of biomolecules were determined. Additionally, the standard batch (macroscale ABS) was compared with flow-through processes (microfluidic setups).

The environmental impact resulting from the release of fluorinated gases (F-gases), used in refrigeration, is instigating the development of technologies to recover and recycle them. FILs and FIL-based DESs were investigated as promising candidates for the absorption and selective separation of three of the most used F-gases in domestic refrigeration (R-32, R-125, and R-134a).[4,5] Further, ILs with high F-gas uptake capacity and selectivity were supported on silica and their potential as media for selective F-gas sorption was studied.[6]

Likewise, the development of ILs and DES that are themselves APIs are building-up platforms with many benefits, including the potential to modulate the water solubility and the membrane permeation properties of an API.[7] The presented results clearly demonstrate that, within the green chemistry framework, a bioprivileged IL and DES platform constitutes a viable alternative for enhancing the bioavailability of poorly water-soluble APIs.

Keywords: ionic liquids, fluorinated ionic liquids, eutectic systems, aqueous biphasic systems, microfluidics, partition, proteins, fluorinated gases, reclamation, porous solid materials, absportion, sportion, active pharmaceutical ionic liquids, active pharmaceutical eutectic systems, bioaivalability.

Acknowlegments:
LIFE Programme of the EU, LIFE-4-Fgases, LIFE20-CCM/ES/001748. FCT-MCTES, Portugal: 2020.00835.CEEIND; PTDC/EQU-EQU/2223/2021; PTDC/EQU-EQU/29737/2017; UIDB/50006/2020 and UIDP/50006/2020.

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Bioprivileged Fluorinated Ionic Liquids in the Purification of Proteins: Towards Enhanced Tunability of Aqueous Biphasic Systems

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Abstract:

The rising number of biomolecules approved by regulatory agencies are driving the global bioseparation market size, forecasted to grow 8.7% annually and reach $14.0 Billion by 2026.[1]

The use of ionic liquids (ILs) in ABS is well established, with outstanding performance in the extraction of targeted biomolecules.[2] We previously proposed cholinium-based ILs as a step towards more benign ABS,[3] disclosed novel ABS composed of fluorinated ILs (FILs)[4] and demonstrated that FILs reduce the impact of the addition of water upon the IL's H-bond acceptance ability.[5] The superior extractive performance of IL-based ABS results from the broad hydrophobic-hydrophilic range exhibited by the coexisting phases when ILs are employed.[2]

In this work, we have explored the full potential of applying FILs, that have emerged recently due to their remarkable performances, [5-7] to widen up the properties and applications of IL-based ABS. Bioprivileged FILs were implemented to develop more versatile and amenable to be tuned ABS. To understand the phase formation process of these novel ABS and their potential as extractive platforms of proteins, the ternary phase diagrams, the coexisting phases' properties (pH, conductivity, viscosity, density and polarity), and the partition coefficients of lysozyme were determined. Further, the stability and activity of lysozyme in the target ABS-phase was also addressed. Finally, to highlight the interactions between lysozyme and the ABS-phase components and better understand the interactions ruling the partition, UV-VIS spectrophotometry, intrinsic fluorescence, nano-differential scanning calorimetry, circular dichroism and microscale thermophoresis measurements were attained.

Keywords: fluorinated ionic liquids, aqueous biphasic systems, lysozyme, partition, stability, activity, UV-VIS, intrinsic fluorescence, nano-differential scanning calorimetry, circular dichroism , microscale thermophoresis.

Acknowlegments:

FCT-MCTES, Portugal: 2020.00835.CEEIND; PTDC/EQU-EQU/2223/2021; PTDC/EQU-EQU/29737/2017; UIDB/50006/2020 and UIDP/50006/2020.

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Characterization and Biotechnological Potential of Extracellular Polysaccharides Synthesized by *Alteromonas* Strains Isolated from French Polynesia Marine Environments

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Abstract:

Marine environments comprise almost three quarters of Earth's surface, representing the largest ecosystem of our planet. The vast ecological and metabolic diversity found in marine microorganisms suggest that these marine resources have a huge potential as sources of novel commercially appealing biomolecules, such as exopolysaccharides (EPS). Six *Alteromonas* strains from different marine environments in French Polynesia atolls were selected for EPS extraction. All the EPS were heteropolysaccharides composed of different monomers, including neutral monosaccharides (glucose, galactose, and mannose, rhamnose and fucose), and uronic acids (glucuronic acid and galacturonic acid), which accounted for up to 45.5 mol% of the EPS compositions. Non-carbohydrate substituents, such as acetyl, pyruvyl, succinyl, and sulfate; and few peptides were also detected. Studies on EPS functional properties revealed that they produce viscous aqueous solutions with a shear thinning behavior and could form strong gels in two distinct ways: by the addition of Fe^{2+}, or in the presence of Mg^{2+}, Cu^{2+}, or Ca^{2+} under alkaline conditions (Figure 1). Moreover the film-forming capacity of the EPS was tested. Results showed that the EPS formed transparent films (Figure 2) with high water vapour permeabilities. Interestingly, the films presented two different behaviors in terms of their mechanical properties under tensile testes: three EPS formed ductile films with high elongation at break (EB), low tensile strength at break (TS) and low elastic modulus (EM); whereas the other three EPS' films showed more stiff and resistant characteristics with a higher TS, low EB and high EM.Thus, these EPS could be versatile materials for different applications.

Keywords: *Alteromonas* sp.; exopolysaccharide; functional properties; rheology; gelation; films

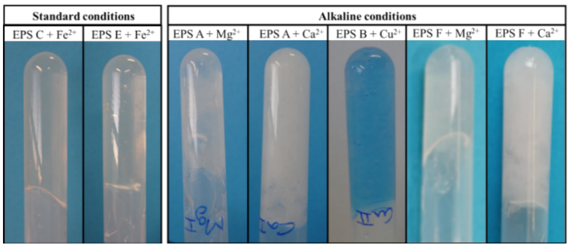

Figure 1: Homogeneous gels that maintained their gel structure in an inversion test formed with different cations, under standard and alkaline conditions.

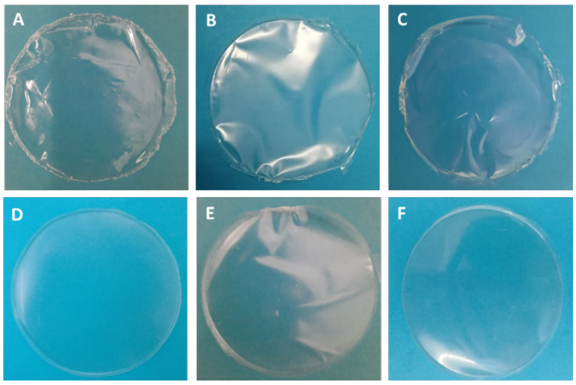

Figure 2: Images of films prepared with EPS produced by *Alteromonas* strains isolated from French Polynesia.

Nano(Bio)Technological approaches for the diagnosis of infectious diseases

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Abstract:

There is increasing evidence that the future of diagnosis will be the analysis of molecular fingerprints defining our state of health. Footprints comprising sets of biomarkers related to the health of our organs, our metabolic state or our microbiota. To accomplish this aim,implementation in clinical laboratories of tools and devices for the detection of multiple biomarkers is mandatory. Multiplexing is the process of simultaneously detecting or identifying multiple biomarkers in a single diagnostic test, which can be valuable for several different types of diseases. For example, pharmacogenomic studies in patients with cardiovascular disease have indicated that the presence of polymorphisms affects patients' response to various drugs. Most cancers have biomarkers in common with other cancers, hence detecting multiple biomarkers is needed for the accurate differentiation of cancer types or location. Infectious diseases are another area where multiplexed diagnostics are extremely valuable.

Most infectious diseases, such as lower respiratory infections, have multiple causative pathogens, but the resulting symptoms do not indicate the causative pathogen and its antimicrobial resistant profile or do not provide enough information for monitoring of the disease, its evolution or its response to treatment. However, multiplexing poses important technological challenges related measurement in a single run of biomarkers of different chemical nature (metabolites, proteins, peptides, nucleic acids, etc.) which can also be present at different concentration ranges. In this communication we will present some nanobiotechnological approaches to overcome these challenges and will focus on the recent advances accomplished in the Nb4D group for diagnosing infections.

Neurological phenotypic nanomedicines: BBB crossing and new therapy development

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Abstract:

The blood-brain barrier (BBB), is the largest brain interface by surface area and allows short diffusion distances (< 10 µm) between blood and neural tissue. The BBB is formed by specialised brain endothelial cells (BEC) whose phenotypic functions are conditioned by the local brain cells, particularly astrocytes and microglia, and mural cells like pericytes and fibroblasts. The BBB plays an important physiological role by tightly gating the passage of ions and molecules, delivering nutrients according to appropriate neuronal needs and, at the same time, protecting the brain from toxins and pathogens. The BBB is a considerable pharmacological hurdle as its impermeability to most drugs limits our developmental capabilities for all neurological disorders.

The problem of targeting is a multifactorial task with non-linear responses to dosing, receptor compositions, and cellular uptake. In the last decade, we have been borrowing tools from statistical and soft matter physics to address such a challenge. We know from the super-selectivity theory (SST) that multivalent units interact via the collective effect of the single affinities (or avidity) and association changes with receptors or ligand numbers not linearly, giving rise to entropy-driven interactions (EDI). This unique nature means that if we combine low-affinity ligands, we can have association only when receptors are high in numbers, effectively targeting cells that overexpress the desired receptor. We and others have proven SST experimentally using either multivalent polymers or synthetic vesicles [1-3]. We showed that by combining the SST design rules with PEG steric control, we could target LRP1 receptors and thus selectively bind and cross the BBB [4-7] or target integrin receptors to deliver chemotherapeutics to cancer cells [8] selectively. We demonstrated that EDIs could be amplified across different ligand/receptor combinations, creating multiplexed targeting solutions [2]. We showed that steric repulsive potentials give rise to non-monotonic association trends with the number of ligands or receptors. The collective affinity can be too low to allow binding at low numbers, whilst the steric effect dominates interaction at a high number of ligands or receptors, hindering any binding [1]. We formalised and experimentally validated such a multiscale theoretical framework to include other natural steric barriers such as the glycocalyx, the polymer brush made of glycosaminoglycan (GAGs) chains surrounding most cells and the dendritic glycans that decorate most proteins.

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Advanced Dynamic Light Scattering and its Application to Life Sciences

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Abstract:
Dynamic light scattering (DLS) is a powerful characterization technique routinely used in research and formulation development in life sciences. It provides a measure of the size of the particles in a suspension, as well as rapid aggregate detection or long-term stability monitoring. Its applications cover a wide range of life science systems such as nanocarriers, proteins, drug products or adjuvants.
While DLS is a well-established characterization technique that provides fast and in-situ information, it is still undergoing constant improvements.
In particular, the notorious need for highly diluted samples has long been a major limitation in DLS. In this context, we will introduce the Modulated 3D DLS technology, allowing to suppress multiple scattering directly in the DLS signal. The measurement of sample at any concentration is thus possible without any limitations.
The access to sizes below 5 nm is another well-known challenge that prevents, among other examples, the accurate characterization of DNA and its conformation changes. This difficulty can be overcome by a different, yet similar improvement of the detection system called the Pseudo-Cross Correlation technique.

This presentation will feature a review of the scientific fundamentals of DLS and introduce the technologies mentioned above.

Keywords: DLS, Dynamic Light Scattering, Characterization Techniques, Life Sciences, DNA, Proteins, Viruses, Nanoparticles, Pharmaceutical, Sizing, Stability, Aggregates,

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Nanotech / Biotech Session II.D: Nanotechnology for life science, Biosensors, Diagnostics and Imaging

Single Polymeric Ion-Conducting Nanochannels as Core of Biomolecular Sensors for Medical Diagnostics

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Abstract:
Analyzing biologically relevant molecules is an important aspect of biomolecular analysis and medical diagnostics. The biomimetic approach presented aims at developing a device that is able to specifically detect and quantitatively analyze (bio)molecules. An example is tumor markers that are emitted by the tumor at elevated levels and can be found in body liquids. If they are discovered in time, more effective countermeasures against further tumor growth can be taken. The core of the analyzing device consists of a polymeric foil containing a single nanochannel. In analogy to biological nanopores that control e.g. mass transfer into and out of a cell, the biomimetic artificial nanochannel allows the passage of ions of an aqueous electrolyte in an electrochemical two-compartment cell from one compartment to the next one under the influence of an electrical field. When the nanochannel wall contains certain immobilized molecules that specifically react with the biomolecule to be analyzed in a key-lock type bioconjugation reaction, the electrolyte-based ionic current *I* is influenced. The difference in the current, taken from current/voltage (*IV*) curves, as a function of the enalyte biomolecul concentration can directly be correlated to the presence and the quantity of the biomolecule to be analyzed.

As examples, the determination of small quantities of histamine (Hm), the well known neurotransmitter that plays a role in inflammatory response, allergies, and immune system functionality, and of phosphoproteins (1) for phosphoproteomics is shown.

Keywords: Biomolecular sensor, nanochannels, microfluidic sensor device, medical diagnostics histamine sensing, phosphoproteins

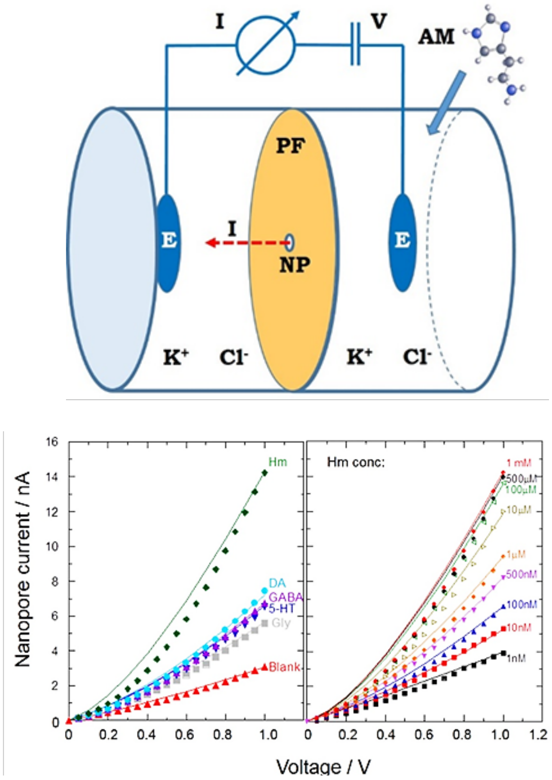

Figure 1: Schematic of electrochemical cell with a central nanochannel for specifically determining a biomolecule, E: electrodes, PF: polymer foil, NP: nanopore, AM: analyte molecule; electrolyte: aqueous KCl solution
Bottom: left: results for histamine (Hm), selectivity of Hm against other neurotransmitters (DA, GABA, 5-HT, Gly), right: quantification of Hm concentration, from 1 mM down to 1 nM.

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WELFA: WAINVAM-E Lateral Flow Assay Innovative and Ultra Sensitive LFA System using the Properties of NV Center Diamonds

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Abstract:

WAINMA-E is a start up which develops a new generation of ultrasensitive and rapid diagnostic test which combines the rapidity of lateral flow immunological assay system with the unique optic and quantum properties of fluorescent NV center-nanodiamonds.

Diamond is a carbon matrix transparent to visible light. In NV centers, a carbon atom is replaced by a nitrogen atom (N) while the neighboring site remains empty (V for vacancy). Because of this, when illuminated with a green laser, the NV diamond emits red fluorescence which is also sensitive to and can be modulated by magnetic field. The surface of nanodiamonds can be functionnalized with various molecules such as antibodies directed against target biomolecules. They can then be used as fluorescent probe in a LFIA system to detect and quantify markers of infection, cancer, inflammation, allergens in a biological matrix. By applying a magnetic field, the reader will create a modulation of the intensity of fluorescence which allows the separation of the nano diamonds signal from the autofluorescence of the support increasing the sensitivity of the detection. It will be possible to detect very low concentrations of biomarkers for an early diagnostic.

Keywords: Nano Diamonds, NV Center, LFIA, Biomarkers, Sensors, Diagnostic

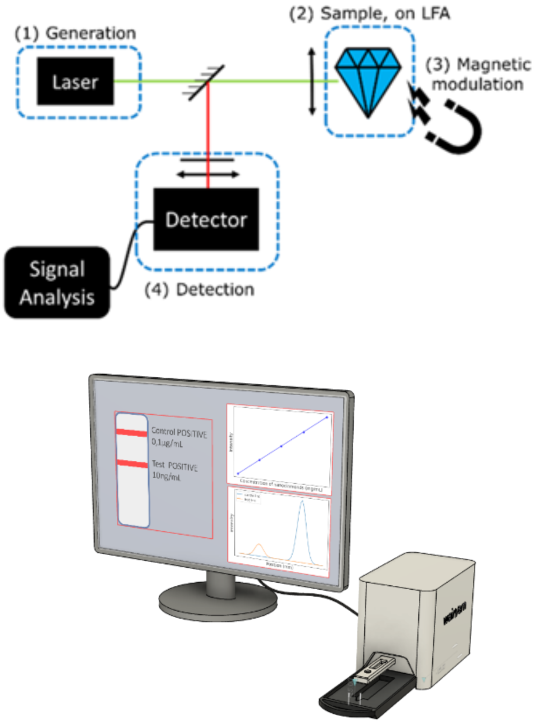

Figure 1: Welfa reader structure

Development of a novel carbonized porous silicon electrochemical sensing platform by pyrolysis of furfuryl alcohol

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Abstract:

Over the years, porous silicon (pSi) has emerged as a promising material, especially in sensing applications, due to its advantageous properties such as a large surface area (>100 m^2/cm^2), ease of functionalization, tuneable pore size (from a few nm to several μm), thickness (from a few nm to the silicon wafer thickness) and porosity. Such features can be easily tuned by simply changing the etching conditions to tailor the desired application needs. Precisely, thanks to its tuneability and versatile surface chemistry, pSi allows the incorporation of a wide range of functionalities for the covalent immobilization of diverse biomolecules as bioreceptors, thereby serving as a perfect tool for biosensing purposes. However, its use as an electrochemical transducer is limited by the chemical instability of hydride terminated freshly etched pSi, that are prone to oxidation. Thus, surface modification of pSi is crucial for its stabilization, while at the same time for crafting desired functional groups on its surface to immobilize various recognition elements.

Herein, we propose the polymerization and carbonization of furfuryl alcohol (PFA) on pSi to get a carbon-stabilized pSi device, featuring a conductive layer as a suitable nanostructured electrochemical transducer. The freshly etched pSi wafers are modified with furfuryl alcohol (FA) by spin coating and later subjected to thermal heating for the carbonization of FA. Morphological features of synthetized PFA-pSi were extensively studied using Field Emission Scanning Electron Microscopy, while Fourier-transform infrared spectroscopy was used to investigate the surface chemistry. Electrochemical characterization using cyclic voltammetry, electrochemical impedance spectroscopy were used to demonstrate the electrochemical performance and stability of PFA-pSi.

Finally, the potential of such platform for electrochemical (bio)sensing applications was underpinned by the development and optimization of a PFA-pSi based biosensor for the detection of bacterial 16SrRNA from *Staphylococcus aureus*. Hence the excellent electrochemical performance of this platform along with its versatile surface chemistry highlights its potential to be used as a novel nanostructured electrode for electrochemical sensing applications.

Keywords: Porous silicon, carbon-stabilization, polyfurfuryl alcohol, electrochemical biosensor

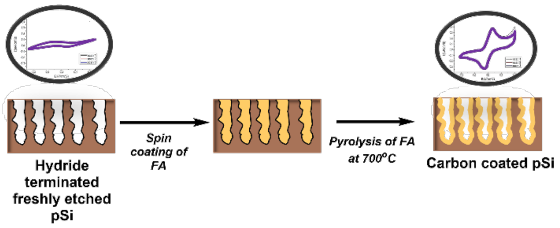

Figure 1: Stepwise carbonization of freshly etched pSi using furfuryl alcohol

References:

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Rapid fabrication of responsive biodegradable microstructures; an introduction to a low invasive research track of multiphoton polymerization for a resolved clinical application

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Abstract:
The fundamental units of living systems are cells, single units with unique geometrical morphology and particular function, that form tissues and organs. Due to the shortage of human derived tissues for implants, there is a large pressure to develop artificial tissues. The tissue regeneration field ideally seeks rapid diagnostics, efficient disease removal, and subsequently regenerating the affected body segment as naturally as possible in a low disruptive way. Since the genesis of the tissue engineering field, many different approaches have been employed to mimic the tissue cellular layouts and molecular compositions (Figure 1). One field that has gained much attention is additive manufacturing. Among various additive manufacturing techniques, the approaches that exploit light, especially laser sources, allowed to reach high spatial resolution in the fabrication of bio-scaffolds, down below the cell size satisfying pre-clinical requirements for native tissue regeneration. However, actual clinical experiments for this precise 3D printing technique will need to address additional constraints like phototoxicity, temporal resolutions, and low responsivity.

Various research groups, like ours, have conducted research programmes to tackle these fundamental limits and requests for micro-structuration through different approaches, from modification in the chemical composition of the resin in use, to the additional responsive dopants or to the optimization of the optical scanning strategies. As an active research track, recently we reported developments in fabrication of biocompatible and responsive microarchitectures made of proteins and featuring variable elastic moduli. The basic micro-models have been created from a proteinaceous ink composing of Bovine Serum Albumin (BSA) and Rose Bengal (RB) by hiring the two-photon-assisted direct laser writing. The generated proteinaceous microarchitectures showed significant biocompatibility, as tested on cells and bacteria cultures. In further practical trials, ink was modified with plasmonic nanoparticles (here gold-branched nanoparticles; GBNPs) to fabricate photothermally-active proteinaceous substrates triggered externally via laser sources with an operating range from visible to near-infrared (NIR). These achievements, making possible to print micro-structures responsive to external triggers, will allow study and guide single cells fate, as demonstrated here on neuron cells whose activity is selectively amplified by irradiation of light and consequent, spatially confined, photothermal effect.

Future efforts in this direction but should also be combined with possible solutions to the challenge of cytotoxicity that is often the drawback of the photo-chemical procedure at the basis of photo-polymerization.

Keywords: Multiphoton polymerization, volumetric 3D printing, proteinaceous microstructures, photothermal effect.

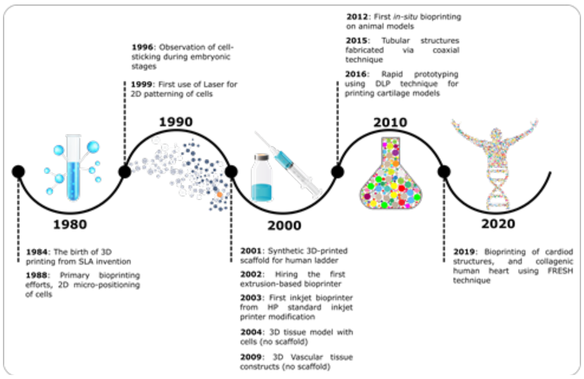

Figure 1: Footprint of 3D printing for human health technology.

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in-vitro Monitoring of Extracellular Matrix Protein Conformations using Gold-Edge-Coated Triangular Silver Nanoplates within a Cellular High-Noise Environment in the Presence of Chitosan Biocompatible Hydrogels

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Abstract:

Several clinical diagnoses rely on the accurate detection and quantification of proteins or peptides for which folding and structure play important roles in the regulation of mechanisms at cellular levels[1]. Misfolding, aggregation or degradation of these proteins can lead to the development of human disorders including neurodegenerative diseases and cancer, among others[2]. At present, the traditional approaches available to characterize and analyse these molecular behaviours in biological systems are remarkably elaborate and their signals are commonly greatly hindered and obstructed by the high background noise of the analysed environment as a result of molecular interactions[3]. The intrinsic high biological noise within biological environments where complex interactions regulate biological processes, poses critical challenges for the study of biomolecular activities significant to advancing approaches to injury and disease treatment. Here we present a straight forward and versatile technique for the study of proteins and their interactions in a cellular environment based on a novel nano-biotechnology method. Highly sensitive gold edge-coated triangular silver nanoplates (AuTSNP) are used to analyse protein behaviours within complex cellular environments in presence of biocompatible tissue regeneration hydrogels. In this work, we present the monitoring of a critical extracellular matrix protein, Fibronectin (Fn), and its dynamic behaviour in its active and denatured forms within the presence of cells (MC3T3-E1 pre-osteoblasts) and chitosan biocompatible hydrogels. The highly sensitive local surface plasmon resonance (LSPR) of the AuTSNP was used to record the Fn over 32 hours upon incubation with cells and hydrogels where large spectral red-shifts were recorded overtime for the active Fn, and limited spectral shifts were observed for denatured Fn. The straight-forward application and outstanding sensitivity of the AuTSNP within biological environments, presents them as powerful new tools to signature protein conformational changes and monitor essential protein behaviours which can provide extraordinary possibilities for the progression of regenerative medicine and assist in disease treatments.

Keywords: Triangular silver nanoplates; protein behaviour; fibronectin, LSPR, hydrogel.

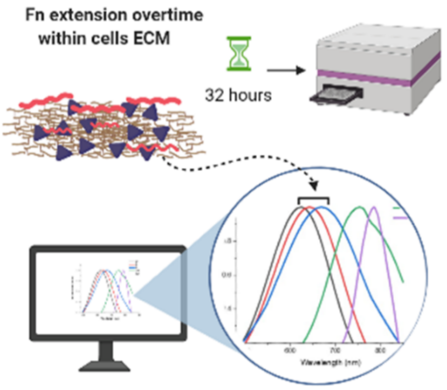

Figure 1: Illustration of Fn monitoring overtime where red shifts in the spectra are recorded as a result of protein extension within the extracellular matrix.

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Self-Assembly of Carbohydrate-based Bottlebrushes in Solution: Glyco-Nanoparticles

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Abstract:

The biological activity of carbohydrates as cell targeting units stimulated an increasing interest in synthetic glycopolymers that are able to target specific cell types, thus, showed great potential applications in infection of pathogens, dectction, signaling and cell-surface recognition[1]. Specifically, hyperbranched bottlebrushes functionized with carbohydrates have attracted considerable attention due to their increasing capability to preventing non-specific protein and bacterial adhesion to coated surfaces compared to their linear analogues[2]. In this context, exerting control over the position and density of maltoheptaose (MH) and polystyrene (PS) pendants attached to a polynorbornene blackbone, several well-defined bottlebrushes (BRs) with different molecular weights were successfully synthesized by M. Mumtaz (Post-doc in the group). Subsequently, a simple method called the solvent diffusion-evaporation-mediated self-assembly[3](SDEMS, Figure 1a), was applied to prepare the homogenous core-shell nanoparticles (NPs) from BRs DMF solution and furtherly diluted into the deionized water. Dynamic light Scattering (DLS), transmission electron microscope (TEM) and atomic force microscope (AFM) were carried out to investigate the structure feature of the obtained nanoparticles. As shown in Figure 1b, upon changing the molecular weight of BRs from 2.3 million, 2.4 million to 3 million, a monomodal and sharp ed` distribution at scattering angles at 90° shifted from 55 nm, 64 nm to 87 nm, which was also consistent with the narrow size distribution of core-shell NPs observed in TEM. At elevated high temperature, the surface morphology of BRs sphere nanoparticles on the hydrophilic modified silicon substrate underwent significant flattening having a tendency to form a cubic (Figure 1c). We anticipated that these discoveries will provide the basis for future studies regarding BRs self-assembly, especially with regard to the morphology formation of nanostructures[4].

Keywords: carbohydrates, glycopolymers, self-assembly, bottlebrushes, core-shell, nanoparticles, cubic shape

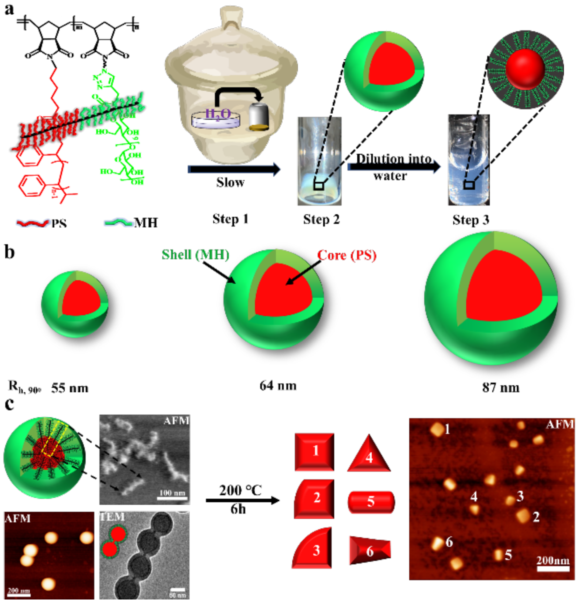

Figure 1: (a) Schematics and photographs of the amphiphilic glycopolymer bottlebrush BRs solution (80 mg/mL, 0.4 mL DMF) and their self-assembly into highly homogeneous core-shell nanoparticles by using SDEMS method and furtherly diluted in to deionized water, (b) effect of molecular weight of bottlebrush BRs on the size of core-shell NPs, (c) Temperature effect on the morphology of core-shell NPs.

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Probing the glycans accessibility of the nanoparticle biomolecular corona

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Abstract:

When exposed to a biological medium, the surface of nanoparticles (NPs) is surrounded by biomolecules, forming the so-called "biomolecular corona" (or corona). It is well established that the corona will represent the new identity of the NPs, affecting their fate in the biological system.

Previous studies have shown that the corona consist of naturally glycosylated proteins, whose glycans have an important role in the NPs interaction with macrophages, but remain unidentified. In addition, it has been demonstrated how the removal of glycans from the corona promotes a pro-inflammatory response and uptake by macrophages. Understanding the glycans composition of the corona is important to predict the NPs toxicity and their behavior in vitro and in vivo.

In this study, we have characterized the corona of gold NPs after their exposure to blood plasma at two different plasma concentrations, mimicking the in vitro and in vivo conditions. We have characterized the biomolecular corona using HILIC chromatography and shotgun proteomics. Afterwords, a lectin binding assay was carried out using Dynamic Light Scattering (DLS) and Fluorescence Correlation Spectroscopy (FCS) to assess whether proteins with known affinity towards specific glycans would bind to the corona.

Our findings highlighted that the protein corona composition is dependent on the exposing conditions, while the glycan composition is comparable, with a prevalence of the biantennary sialylated glycans (A2G2S2). We confirmed that the glycans are accessible for binding as the corona interacts with lectins with known glycan affinity, while the enzymatic removal of the glycans leads to a decrease in lectin affinity. This study shows for the first time that the glycans are present in the corona and that they could potentially be responsible for the modulation of NP biological processes as they can directly engage with glycan binding receptors that are highly expressed in an organism.

Keywords: Biomolecular corona, glycans, lectins, Fluorescence Correlation Spectroscopy, proteomics, Gold Nanoparticles.

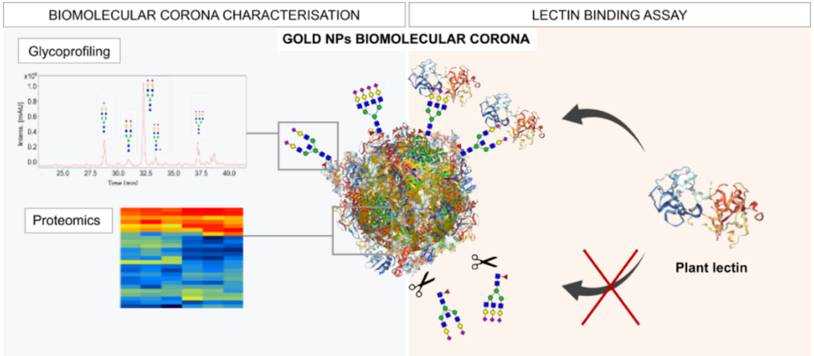

Figure 1: Summary scheme of the project. Gold nanoparticles were incubated in human plasma to form a protein corona, deeply characterized through proteomics and glycan analysis. The accessibility of the glycans was explored using plant lectins.

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Gold nanoparticles long-term evaluation in liver: role of shape, size and surface functionalization

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[4] INGM Imaging Facility, Istituto Nazionale Genetica Molecolare, Milano, Italy.
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Abstract:

Correlation among physicochemical properties of plasmonic nanoparticles (NPs) with their interactions in biological matrices is key for nanomedicine. One of the main issues is the uncertainty regarding nanomaterials behaviour in humans body and other animals, due long-term accumulation. While biodistribution of NPs has been widely studied at organ levels, little is known about their accumulation in organs at subcellular level. Since the liver is the main filter organ for NPs, this work was aimed at evaluating hepatic accumulation, internalization and safety of NPs in healthy mice after a single administration for short- and long-term periods. Herein, we compare the influence of shape, size, polymer coating and glycan functionalization on their fate in the hepatobiliary clearance using ICP-MS combined to advanced microscopy. Our data demonstrated that geometry and surface functionalization can dramatically change liver kinetics. Ultra-structural analysis showed that NPs were rapidly segregated into lysosomes of endothelial cells (LSEC) or Kupffer cells independently on their physicochemical features. We have further demonstrated the biocompatibility of gold NPs coated with sialic acid glycopeptides (glyco-NPs) and its ability to reduce liver uptake but exclusively in rod-like shaped NPs.

Overall, this study can be conisedered a platform to predict the subcellular disposition in organs after short- and long-term periods and the impact of glyco-NPs on their biological fate as an engineering tool for the designing of nanomaterials towards clinical translation.

Keywords: plasmonic nanoparticles, glycopeptide, kupffer cell, endothelial cell, lysosomes, cellular internalization

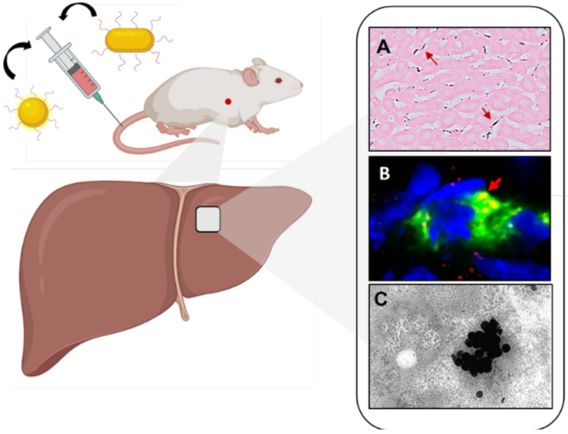

Figure 1: Long-term accumulation of gold NPs at a subcellular level in liver. A) Histological evaluation of gold distribution (black spots) in liver tissue by AMG. B) NPs co-localization with Kupffer cells by reflective SIM. C) Ultrastructural localization of NPs inside liver cells by TEM.

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Exploring the Synthesis Conditions for Magnetic Pd/Fe-oxide Nanoparticles

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Abstract:

In recent years, research has increasingly focused on the production of complex multifunctional heterostructured nanoparticles (NPs) that can combine two or more different inorganic species in a single component. These nanosystems have an immense potential for a multitude of applications because of the ability to combine the properties of multiple materials in a single entity. However, the properties of such nanomaterials are in strong correlation with their size, morphology, and other structural specifications. Therefore, enormous efforts were devoted to achieving high and precise control over the synthesis of such materials. [1]

We report an example of such nanomaterial, a Pd-iron oxide hybrid nanoparticle. These heterostructures were synthesized by thermal decomposition via a straightforward, classical one-pot synthesis method, where homogeneous nucleation and seed-assisted growth occur simultaneously, and also via a seed-mediated method, where the heterogeneous nucleation and growth of a second solid phase take place on the surface of preformed so-called "seeds" introduced in the reaction mixture (Figure 1). [2,3]

In the case of the latter synthesis method, we additionally investigated the effect of different reaction parameters on the outcome of Pd/Fe-oxide NPs by systematically changing parameters such as the iron precursor/Pd seed ratio, functionalization of the Pd seeds, surfactant/Fe ratio, heating rate and solvent. Until now, the few studies on Pd-iron oxide existent in literature focus on catalysis as main application. However, we believe these hybrid NPs have great potential in other applications such as biomedicine, due to their magnetic properties. Therefore, we focused through our study on defining the optimal conditions to produce Pd/Fe-oxide nanocrystals that offer the best magnetic properties, which make them great candidates for hyperthermia/thermal ablation and MRI visualization.

Keywords: heterostructured nanoparticles, thermal decomposition, one-pot synthesis, seed-assisted growth method, magnetic properties, catalysis, biomedical applications, hyperthermia, imaging.

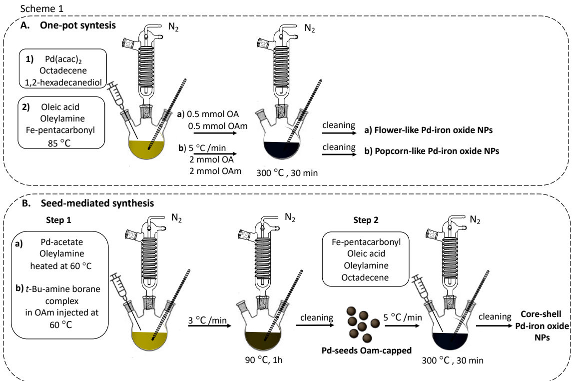

Figure 1: Synthetic routes for the preparation of hybrid Pd/Fe-oxide NPs via **(A)** one-pot procedure and **(B)** seed-mediated synthesis.

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Polyhydroxyalkanoates (PHAs) and FucoPol based scaffolds for tissue engineering applications

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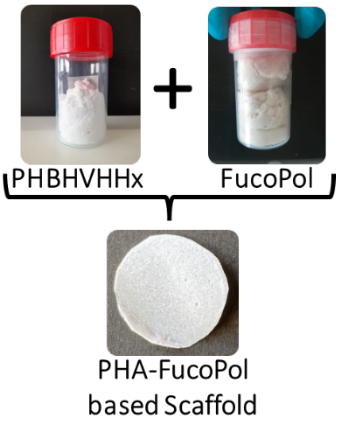
Abstract:

Poly(hydroxyalkanoates) (PHAs) are produced inside bacterial cells as carbon and energy storage compounds. Depending on the number of carbon atoms of their monomers, they can have different properties, ranging from brittle and rigid thermoplastics (e.g. poly(3-hydroxybutyrate)), to flexible and elastomeric polymers (e.g. poly(3-hydroxyoctanoate-co-3-hydroxydecanoate))[1]. On the other hand, exopolysaccharides (EPS) are high molecular weight carbohydrates secreted by bacterial cells, or bonded to their surface, to provide protection against environmental stress, cell adherence to surfaces and carbon or water storage reserves[2]. Due to their inherent biodegradability, biocompatibility, structural and chemical properties, PHAs and EPSs are attractive raw materials which can be processed to fabricate structures, such as films or gels, as part of scaffolds for tissue engineering. Some EPSs, such as the fucose-containing bacterial polysaccharide FucoPol, possess biological activity (e.g., wound healing and photoprotective capacity) that can improve the biological performance of these scaffolds. The main goal in this work was to produce a PHA-based 3D structures with enhanced hydrophilicity and cell adhesion ability. To achieve this, a PHA terpolymer composed of 69 wt% 3-hydroxybutyrate, 24 wt% 3-hydroxyvalerate and 7 wt% 3-hydroxyhexanoate (P3HB-3HV-3HHx) was used to produce a porous film by an emulsion templating technique with a FucoPol aqueous solution. The resulting porous films had a Young modulus of 85 MPa, a tensile strength at break of 4.4 MPa, together with an elongation at break of 52%. This work demonstrated the potential of PHA-FucoPol based scaffold to be used for tissue engineering applications.



Keywords: tissue engineering; PHA-based scaffolds; poly (3-hydroxybutyrate-co-3-hydroxyvalerate-co-3-hydroxyhexanoate) (P(3HB-3HV-3HHx)); Exopolysaccharides (EPS); FucoPol

Figure 1: Schematic representation of PHA-FucoPol based scaffolds.

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NanoMatEn / GAMS Joint Session III.A: Materials and Nanomaterials for Energy / Nanoelectronics/ Nanophotonics

Chipless Electronics: a Sustainable Commitment beyond Silicon

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Abstract:
Currently, interface electronics for communicating and storing data is a key issue to serve a plethora of applications, such as security applications and for the internet of things (IoT) that is growing and so, demanding more data to be handled. This has been pushing to the limits the use of silicon for a broad range of applications that can be easily replaced, for which speed of data transmission or storing is not a limiting factor. Moreover, more and more sensing devices are required to support security actions, comfort, and welfare for all, mainly using conformable low-cost substrates. Metal oxides at a nanoscale, together with printed electronics can answer to most of these demands, reverting the push to the need for silicon chips by exploiting green technologies sustained by abundant materials, leading so to the reduction of carbon footprint, and paving the way for green electronics. In this presentation, we will focus on the recent developments on these issues made at CENIMAT.

Structural color in ordered and disordered photonic media

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Abstract:
Different from color from absorbing pigments, structural color arises from spectrally selective scattering. Both 3D-ordered photonic crystals and disordered photonic glasses from spherical particles show potential as structural color. The fact that the coloration effect stems from the scattering properties, thus the refractive index and the size and arrangement of the particles, rather that specific electronic transitions as in pigments creates an independence in the choice of materials, e.g., allows to use non-toxic materials like ceramics and glasses which also are insensitive to UV-bleaching under sun light. We will present the underlying mechanisms of color formation, e.g. the intricate interaction between lattice and motif properties in real and reciprocal space and the role of the Fresnel reflection at the interfaces of film-like structures. Different mechanisms can be responsible for structural color formation depending on the part of the visible spectrum. Blue structural color is widely present in nature and can also be realized with artificial photonic media, e.g., angle independent in disordered photonic glasses. Via Fourier-space engineering we will demonstrate how the saturation of blue structural color can be enhanced using core shell particles. On the other side of the spectrum red colors in nature are mostly pigment based. Red structural colors are difficult to achieve as shorter wavelengths of the visible spectrum are usually also strongly scattered which ruins the color saturation. We will also discuss how selective light trapping in a layer of photonic glass in combination with broadband absorption can pave a route to obtaining a red structural color.

Keywords: Structural Color, Selective Scattering, Disordered Photonic Media

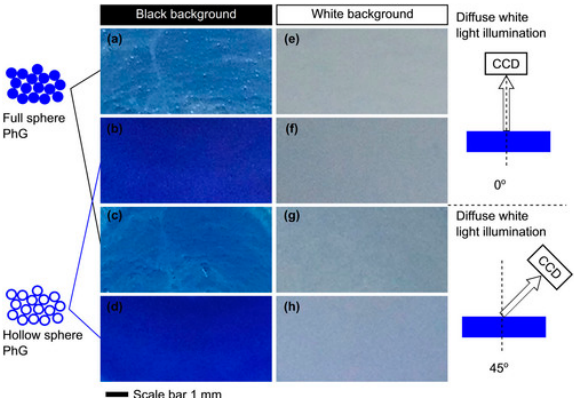

Figure 1: Color impressions of the polystyrene (PS) full sphere and yttria stabilized zirconia (YSZ) hollow sphere photonic glass (PhG). The color expressions of the PS full sphere PhG (a) and YSZ hollow sphere PhG (b) viewed at an angle of 0° [(a) and (b)] and 45° [(c) and (d)], respectively. Images in each row represent the same sample with black [(a)–(d)] or white [(e)–(h)] background. The digital images of cm sized films of the PS full sphere PhG and the YSZ hollow sphere PhG are taken simultaneously to ensure the same diffuse illumination and viewing conditions for the color comparison.

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Correlating the functional properties of graphene on the nanoscale

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Abstract:

The industrial application of graphene in high-performance nanoelectronics requires wafer-scale fabrication, ideally on insulating substrates, and electronically uniform surface properties [1]. Therefore, real-space imaging of the graphene topography as well as mapping the electronic properties with a nanometer resolution is essential. Atomic force microscopy (AFM) not only visualizes surface topography, but can additionally resolve functional properties, such as surface potential and work function, adhesion and elasticity.

Here, we investigated electronic and mechanical properties of a CVD grown wafer-scale graphene film on sapphire [2] via functional AFM techniques. Using sideband Kelvin probe force microscopy (KPFM) we were able to resolve a heterogeneous surface potential distribution with distinct contrast between the bulk film, graphene wrinkles as well as on the underlying sapphire terraces and step edges [3]. The surface potential distribution correlated with the mechanical behavior, including deformation and adhesion, which gave a distinct contrast on the same features, resolved via PinPoint nanomechanical AFM. The correlation of the surface potential and the sample's nanomechanical response may originate from a delamination at step edges, affecting the local electronic properties. Especially the local change of the surface potential has to be considered when incorporating graphene in nanoelectronic devices.

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Figures

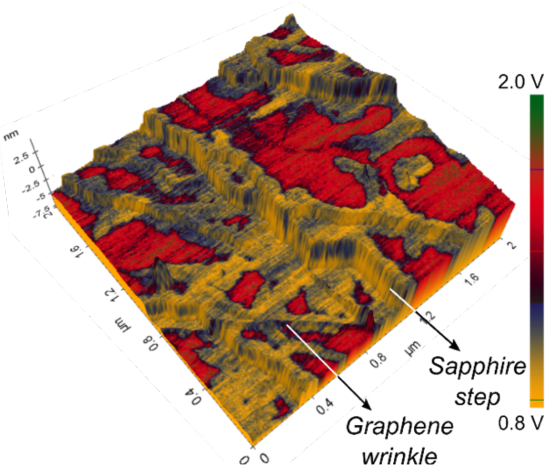

Figure 1: 3D overlay of the graphene topography, which displayed wrinkles and underlying sapphire steps as indicated, with the surface potential imaged via sideband KPFM.

Exploring Memristive Squaraine Microtubes: Programmable Multi-Level Memory Behaviour for Neuromorphic Applications

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Abstract:

Typically, the demand for faster, cheaper, more efficient computing has been answered by device miniaturisation. However, device down-scaling (particularly that of transistors) is fast approaching the atomic scale, resulting in a gulf between the computational efficiency required by data scientists and hardware capacity available from conventional computing based on the von Neumann architecture and binary operations.[1] Artificial electronic synapse (e-synapse) devices are necessary in order for the effective implementation of artificial neural networks (ANNs) in hardware / machine learning operations to occur.[2] Organic memristors can provide the functionality required to meet these computational demands by providing multi-level memory coupled with high-density integration, as well as possessing all of the advantages inherent to organic materials such as flexibility and biocompatibility.[3] Memristors are two-terminal resistive switches which can encode information in the form of programmable internal resistance, the evolution of which can be modulated by the history of its external stimuli.[4] Memristors offers much greater memory density than typical devices by enabling 'multi-bit' memory, as well as facilitating the co-location of memory and logic operations, overcoming the energy- and time-expensive separation between memory and computation execution.[5]

Herein we demonstrate self-assembled microtubes (MTs) with analog resistive switching / programmable multi-level memory based on 2,4-bis[4-(N,N-diisobutylamino)-2-6-dihydroxyphenyl]squaraine (SQ(OH)$_2$), a small-molecule organic semiconductor. The device shows the typical pinched hysteretic *I-V* loop of a memristor with gradual changes in conductance upon successive sweeps, akin to the synaptic weight update processes in the human brain. The memory retention is shown to decay to its original state within a relatively short time in the absence of external voltage application, which is satisfactory for neuromorphic computing applications such as online learning where the synaptic weight values can be stored elsewhere following the training process.[2] This time-dependence enables short-term plasticity functionality to be demonstrated (paired-pulse facilitation and post-tetanic potentiation). Potentiation and depression cycles are shown to exhibit linear and symmetric conductance tuning, a key requirement for implementation of neuromorphic computing. Furthermore, short-term memory to long-term memory conversion is demonstrated through repeated sequences of voltage pulses. Overall, SQ(OH)$_2$ MTs appear to present attractive properties that could enable the successful embedding of organic MT-based ANNs directly in hardware circuits.

Keywords: squaraine, microtube, memristor, analog, neuromorphic

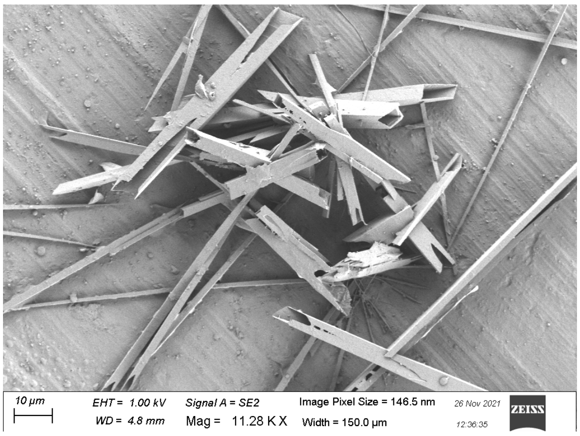

Figure 1: SEM image of SQ(OH)$_2$ MTs.

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Parametric spinwave excitation and mode control using built-in current in a NiFe nanowire

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Abstract:
Parametric pumping is a nonlinear wave phenomenon and a promising technique for electronic devices based on spin waves, so-called "magnonics". For parametric excitation, a a 650 nm-wide NiFe nanowire that has a built-in dc current line to produce an Oersted field is designed, and for spin wave detection, a micro-Brillouin light scattering (μ-BLS) system is used. A spin wave with a frequency of f_{sw} = 5.6 GHz is observed when a pumping microwave with a frequency of f_{mw} = 11.2 GHz is applied. Figure 1 shows the threshold characteristics of spin excitation as a function of the field, where the threshold values are observed to follow an asymmetric butterfly curve.The wave is found to be of the n = 1 width mode (n is the antinode number), and its mode changes to an edge-localized (or possibly $n > 1$) mode when the Oersted field (or current) varies. Joule heating effects are not observed in the pumping process. Thus, spin wave mode control by the built-in current would be a convenient and useful method to enhance the efficiency and compatibility in applications of spin-based electronics.

Keywords: spin excitation, spin wave, parametric spin pumping, magnetic nanowire, Brilloin light scattering, magnonic applications.

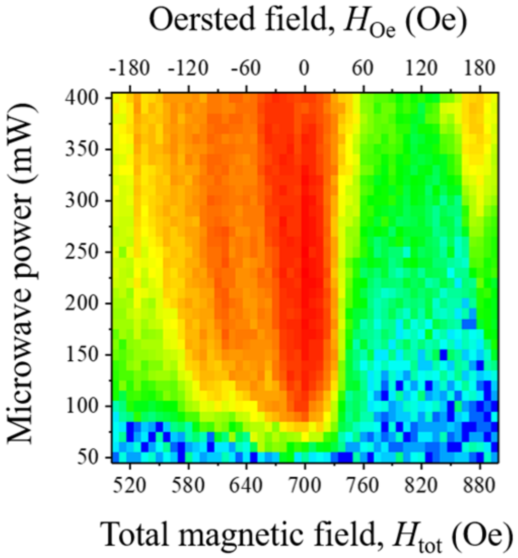

Figure 1: Threshold characteristics of parallel parametric pumping, i.e., BLS intensity as a function of the microwave power with a fixed frequency (f_{mw} = 11.2 GHz) and the magnetic field: the Oersted field and total field are controlled by the dc electric current. The color scale represents the BLS intensity of the spin wave with a frequency of f_{sw} = 5.6 GHz.

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Nonlinear optical thermometry based on Upconversion Luminescence and Second Harmonic Generation (SHG)

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Abstract:

It is well known that non-linear optical (NLO) spectroscopy may be a powerful tool for optical sensing of various intrinsic properties of materials and different state functions of the system. This is related to the strong dependence of non-linear phenomena on numerous physicochemical factors. In addition, the feasibility of simultaneous applying the second harmonic generation (SHG) and upconversion luminescence (UCL) processes in two upconverison systems, i.e., Ho^{3+}, Yb^{3+}, as well as Er^{3+}, Yb^{3+} in $BaTiO_3$ host for optical temperature sensing is demonstrated. Under 976 nm laser excitation, the evolution of SHG and UCL band intensity ratio was correlated with temperature and calibrated within the temperature range of interest The band intensity ratio between SHG and UCL exhibits a sigmoidal dependence on temperature, and, hence, it can allow the detection of phase transitions from non-centrosymmetric to centrosymmetric systems, and vice versa. Importantly, from the perspective of optical temperature sensing, this work provides a novel and effective strategy for non-linear optical thermometry, with high sensitivity.[1] In addition, in the Er^{3+}, Yb^{3+} doped $BaTiO_3$, the thermometric performance of NLO method are compared to that of the converional Boltzmann thermometry, indicating NLO thermometry shows much better relative sensitivity and temperature resolution. [2]

Keywords: non-linear optical thermometry; second harmonic generation; upconversion luminescence; $BaTiO_3$ material.

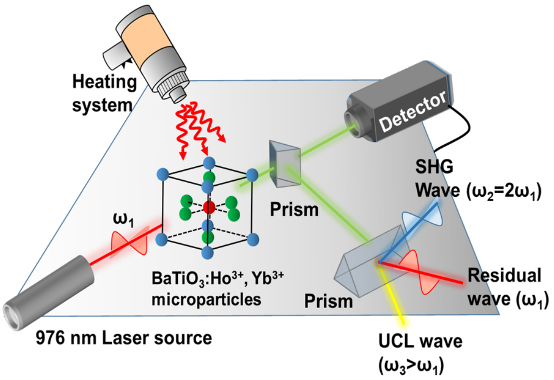

Figure 1: Schematic representation of the experimental setup for non-linear optical thermometry.

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Synthesis of tunable nano-lamellar transition metal hybrid materials and their behavior as battery electrode materials.

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Abstract:

Over the past 30 years, there has been a growing demand for batteries in terms of production and performance. It is therefore essential to develop new types of batteries that meet these societal challenges. For this purpose, nano-organized materials seem to be a promising option. Indeed Chan *et al.* showed differences in performance depending on the nano-structure of cobalt oxides.[1]

The development of hybrid materials is a key step in many fields of research allowing the understanding of various phenomena. These organic-inorganic materials structured at different scales (micrometric, nanometric) can be elaborated by a method already developed in the laboratory.[2]

This thesis work focuses on the synthesis of nano-organized hybrid materials based on transition metals, intended to be used as battery electrode materials.

These materials are realized via robust and reproducible solvothermal syntheses, which involves mixing a transition metal and a bridging ligand (dicarboxylic acid) in a Teflon autoclave (Parr©). The hybrid materials are obtained (figure 1) in the form of very thin sheets made up of nano-lamellae (alternating organic and mineral fringe) with an interlamellar distance of approximatively one nanometer (this value is observed by HRTEM/electron diffraction/XRD/SAXS analysis). These new materials are characterized *via* elemental analysis of C/O/N, ICP-OES, XPS, IR-Raman spectroscopy and TGA-MS allowed to show a first estimation of the formula: $(Co(OH)_2)_{5/3}NDC_2OAm.xH_2O$. (With NDC for 2,6-naphthalendicarboxylate and OAm for Oleylamine).

This type of material seems interesting, as it is expected to allow a better diffusion of the cation (Li^+) in the electrode, du to there peculiar structure.

The first performance tests are scheduled for early this year.

Keywords:

Nano-material, nano-lamellae, bridging ligand, solvothermal, Cobalt-based hybride material, battery applications.

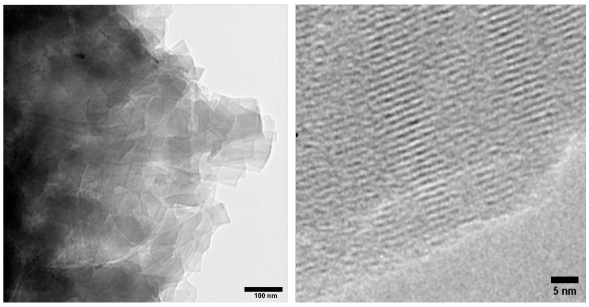

Figure 1: Pictures TEM of nano-sheets (left) and HRTEM on single nano-sheet (right)

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InN on Si(100) photovoltaic devices with an amorphous Si interlayer deposited by DC and RF sputtering

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Abstract:
III-nitride materials have gained great interest in the past decades due to their potential applications in visible-NIR optoelectronic devices, in particular in photovoltaic applications. Recent studies demonstrate that InN-based heterojunctions are a promising technology for solar devices with an impact on space applications [1].

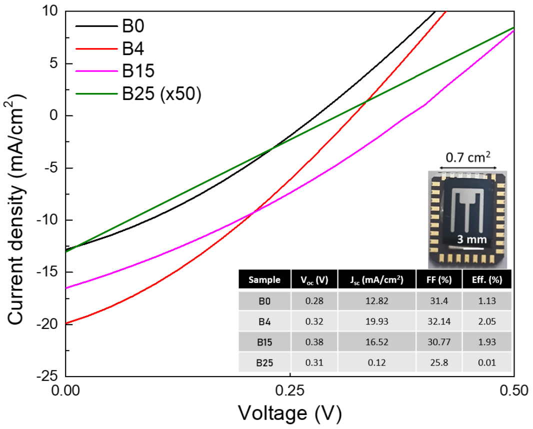
In this work, we study the influence of a Si buffer layer on the material and electrical properties of InN on Si(100) photovoltaic devices deposited via DC-RF sputtering. The Si buffer was deposited by DC sputtering with different deposition times, obtaining a nominal thickness of 0, 4, 15 and 25 nm (samples B0, B4, B15 and B25, respectively). These deposition conditions were previously optimized (see another abstract of the same author) and led to compact amorphous silicon (a-Si). Then, ≈260 nm of InN was deposited, which optimized conditions can be found at [1].

X-ray diffraction data of the InN/a-Si/Si(100) structures show a wurtzite structure oriented along the *c*-axis for all samples, without phase separation. The FWHM of the θ-2θ diffraction pattern of the InN(0002) remains unaltered by the introduction of the Si buffer interlayer, pointing to InN material with the same structural quality with and without buffer layer. Optical transmission spectra measured on InN samples co-deposited on sapphire show a similar apparent bandgap energy of ~1.7 eV (729 nm), as expected from their high residual carrier concentration [2].

Devices of ~1 cm^2 size area were processed using the InN on Si(100) heterojunctions with the n- and p-contacts formed by 100 nm-thick Al deposited by DC sputtering. Then, current density-voltage (J-V) curves were measured in the dark and under 1 sun of AM1.5G solar illumination to obtain the diode and photovoltaic characteristics of the devices. From the analysis of the dark J-V curves, we observe an increase of the series and shunt resistances with the Si interlayer thickness and a minimum J_0 for the sample with 4 nm of Si buffer. This is probably due to the reduction of recombination centers at the nitride/a-Si interface thanks to the unbundling of the nitride layer from the commercial Si substrate. This improvement can be also observed from the analysis of the illuminated J-V curves, in which the open-circuit voltaje increases from 0.28 V to 0.38 V from samples B0 to B15, respectively; while the short-circuit current density shows a maximum of almost 20 mA/cm^2 for the InN sample with 4 nm of Si buffer layer. Both effects result in a FF of 32%, leading to a maximum efficiency of the device of 2.05% for the sample with 4 nm of a-Si buffer (sample B4). However, increasing even more the a-Si buffer thickness kills the electrical characteristic from the heterojunction in the dark and under illumination.

These results show the use of sputtered a-Si as a potential candidate for a buffer layer to increase the photovoltaic performance of III-nitride devices, wherein in this case there is a stunning 80% increase in overall conversion efficiency (from 1.13% to 2.05%).

Keywords: Indium Nitride, silicon interlayer, DC and RF sputtering, solar cell device.



Sample	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	Eff. (%)
B0	0.28	12.82	31.4	1.13
B4	0.32	19.93	32.14	2.05
B15	0.38	16.52	30.77	1.93
B25	0.31	0.12	25.8	0.01

Figure 1: Current density vs voltage curves of the InN on Si(100) devices under AM1.5G illumination (1 sun) vs the a-Si buffer thickness. Inset: table summary of fotovoltaic parameters of the devices and top-view photograph of a representative device.

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Trichalcogenide materials for small bandgap photovoltaic devices

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Abstract:
Solar energy is the most abundant renewable energy resource available to us. Efficient utilization of solar energy requires the coordinated action of a variety of light absorbers with different absorption thresholds. Common photovoltaic (PV) technologies use materials with an absorption threshold of 1.1-1.5 eV, which uses only a limited portion of the solar spectrum. Coupling an infrared PV device with a bandgap of 0.6-0.7 eV to standard PV technologies can improve overall power conversion efficiency by 5-11%. However, for the near/mid-infrared region, there is a limited variety of light absorbers, such as Ge (E_g = 0.66 eV) and GaSb (0.72 eV), which are expensive to make. V2VI3 trichalcogenides, such as Sb_2Se_3, possess a large absorption coefficient (~10^5) and a long diffusion length of 1.7 micrometers along the hk1 direction. In addition, it can be alloyed with Bi to narrow the bandgap and match with other light absorbers. Moreover, the quasi-one-dimensional crystal structure of V2VI3 trichalcogenide materials is supposedly self-passivated due to the closed-shell chemical structure of the grain boundaries. These properties make these materials attractive for small bandgap PV applications. In this work, we have developed two techniques for synthesizing $Bi_xSb_{2-x}Se_3$ alloys for PV. The first technique is a benign solution process approach, and the second is a close-spaced sublimation. We successfully incorporated Bi (up to 40 %At) without forming any secondary phases. As a proof-of-concept, we have also prepared solar cells with an absorption edge extended from 1050 nm to 1150 nm with 12%At. Bi content. Further incorporation of Bi extended the bandgap to 1370 nm. These new techniques can be later used to tune the bandgap and eventually form low-cost multiple junction solar cells.

Keywords: Small bandgap; photovoltaics; self-passivation;

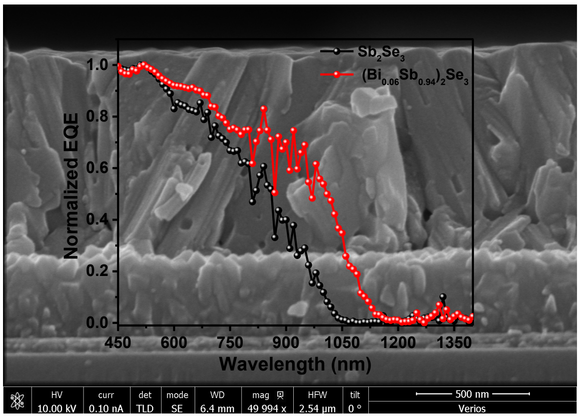

Figure 1: Cross-section SEM image of Sb_2Se_3 overlaid with normalized external quantum efficiency plot of Sb_2Se_3 and $Bi_xSb_{2-x}Se_3$ photovoltaic devices.

2D Organic-inorganic perovskites for next generation optoelectronics

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Abstract:
Fast signal processing devices working at the interface between photonic and electronic systems are required to have large bandwidth real time photoresponse, high sensitivity and be capable of operating at ambient condition. These performance requirements impose stringent requirements on the electrical and optical properties of materials, with only a few systems passing the threshold. The new emerging class of layered 2D organic-inorganic perovskites are attracting growing attention owing to their unique combination of photophysical and electrical transport properties. [1-5] However, their instability to ambient conditions and solvents used in device fabrication have so far hindered their potential for signal processing technologies. In this talk I will discuss a reliable way to enhance the resilience of these materials and demonstrate top-down semiconductor processing of high-quality nanoscale structures based on them. Hence, I will present a detailed characterization of the opto-electronic properties of 2D perovskite devices, and demonstrate that their performance exceed that of high-end commercial Si and InGaAs-based structures. Finally, I will demonstrate the use of 2D perovskite opto-electronics in a range of imaging applications.

Keywords: 2D materials, Inorganic-organic hybrid perovskites, optoelectronics, electron beam lithography.

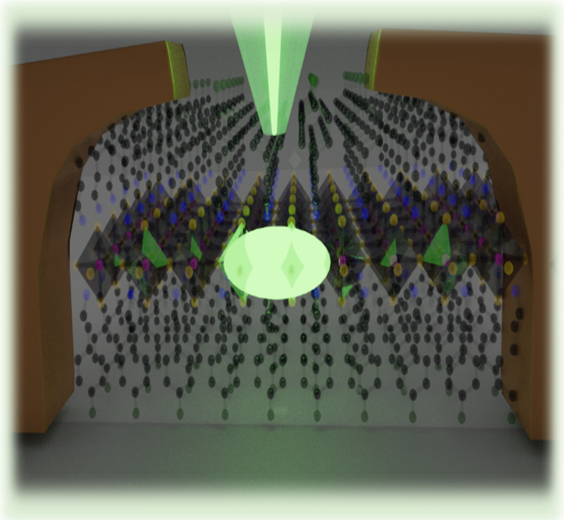

Figure 1: Figure depicting an incident light beam generating an exciton in a 2D hybrid perovskite crystal with patterned electrodes.

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Photoexcitation dynamics and long-lived excitons in strain engineered transition metal dichalcogenides

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Abstract

Two-dimensional (2D) monolayers of transition metal dichalcogenides (TMDs) provide atomic scalability and a host of interesting and useful properties for novel optoelectronic applications, one being the emergence of direct bandgaps in many MX_2 (M- Mo or W; X – S or Se) materials at the monolayer limit. Being at the atomic layer limit, TMD monolayers are strongly dependent on the local environment and growth conditions. In particular, strain has been identified as having important influence on the electronic band structure and optical properties of TMDs that could drive an indirect-to-direct bandgap modification in a large majority of 2D monolayers. In lieu of epitaxial growth, strain-engineering efforts have focused on the growth of high-quality TMDs on glassy substrates (sapphire, silica, *etc*.). Various amounts of strain are obtained by utilizing mismatches in the thermal coefficients of expansion between the substrate and the TMDs as well as by varying processing conditions (high temperature, rapid cooling). Several recent works have studied the effect of the growth substrate on the PL emission characteristics, implicating the influence of bright excitons. Surprisingly little, however, is known about the strain influence on the relaxation dynamics of indirect excitations, expected to be revealed in the dynamics of transient absorption (TA) response. Here, we explore the transient dynamics in a series of TMD monolayers (WS_2, WSe_2, MoS_2) grown on fused silica substrates by the recently developed laser-assisted synthesis technique (LAST). The direct laser vaporization from stoichiometric powders done at the high vaporization temperatures (e.g. ~1400°C for MoS_2) produces nearly defectless, large-area monolayer flakes that are free of contaminants typically found in CVD flakes when various precursors and gases are employed. Consistent with the expectations for the strain-induced band modifications, we observe red-shifted absorption and PL emission signatures as compared to TMDs grown by traditional methods. Femtosecond TA response reveals red-shifted bleach signatures as well, with shifts approaching 0.2 eV for MoS_2 samples. Furthermore, upon an increase in the excitation fluence, decay dynamics of the main TA bleach become progressively longer, reaching several nanoseconds, in marked contrast with commonly observed decay patterns in conventional TMDs. With the help of kinetic modeling, we rationalize our observations as resulting from strain in as-grown samples and corresponding modifications of the electronic bands of the monolayers. With the modified band structure, indirect intervalley K-Γ excitons become low-energy excitations to compete with conventional intravalley excitons. This opens new relaxation channels and changes the overall relaxation dynamics. As illustrated with the model rate equation analysis, the resulting effective partitioning into direct and indirect exciton channels can account for the observed fluence-dependent population dynamics at both short and long timescales. The dark intervalley excitons thus provide for longer-lived system photoexcitations. These findings should provide important insights into the influence of the growth conditions on the nature of optical excitations and their relaxation for future applications of monolayer TMDs. They also call for more detailed studies of the density-dependent competition between different relaxation and decay routes in TMDs, including different valleys that go beyond the quasi-static picture of electron-electron interaction effects.

NanoMatEn - Session III.B : Nanotechnology for Energy / Nanocatalysis (Part I)

Boosting 2D semiconductors with molecules: high performance multi-responsive electronic devices

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Abstract:
Two dimensional materials display outstanding physical and chemical properties which can be further enhanced and enriched through the controlled functionalization with molecules and their assemblies thereof yielding hybrid systems with programmed characteristics for applications in (opto)electronics, sensing and energy. Molecules can be designed and synthesized to controllably physisorb or chemisorb onto 2D materials. [1]

In my lecture I will review our recent findings on the functionalization of 2D materials to engineer hybrid systems via:

- *physisorption* of molecular switches onto the two surfaces of scotch tape and CVD 2D semiconductors, by mastering a Janus approach, to impart additional properties to WSe_2, rendering the 2D material-based transistors capable to respond to four different independent stimuli.[2]

- *chemisorption* of dithiolated molecules onto solution-processed semiconducting TMDs to simultaneously heal sulfur vacancies in metal disulfides and covalently bridge adjacent flakes, thereby promoting percolation pathways for charge transport, leading to a 10-fold increase in field-effect mobility, I_{ON}/I_{OFF} ratio, and switching times of liquid-gated transistors.[3]

Our modular strategies relying on the combination of 2D material with molecules offer a simple route to generate multifunctional coatings, foams and nanocomposites with pre-programmed properties to address key global challenges in electronics, sensing and energy applications.

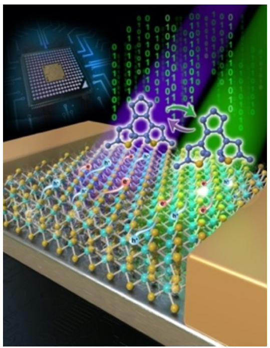

Figure 1: Optically switchable multilevel high-mobility FETs based on few-layer ambipolar WSe_2.

Figure 2: 1,4-benzenedithiol molecules healing sulfur vacancies in solution-processed MoS_2 and covalently bridging adjacent flakes, to create percolation pathways for the charge transport in FETs.

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Bio-Inspired Materials for the Energy Challenge of the Century

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Abstract:
We are facing the contemporary challenges of the impacts of human activities such as the climate change induced by the increase of CO_2 emission since the Industrial Revolution. The nuclear approaches is a way to remedy this situation, both the fission-based and fusion-based. One of the challenges of fission nuclear path is its radioactive spent nuclear waste that can accumulate for more than the civilizational epoch.[1]

This work is a contribution to the design and realization of a Molten Salt Reactor (MSR) (FLiBe) in the size of what is generally called SMR (Small and Medium Reactor). The goal of the reactor is to eliminate the long-life nuclear elements from the nuclear waste that is the minor actinides. Neutronic transmutation of the spent fuel will reduce the amount of trans-uranium elements in the molten salt.

Reactions in a transmutation reactor produce a high population of neutrons which have deterious effects on surrounding materials especially for the first wall of the reactor in contact with the molten salt.

This work proposes to design and produce a bio-inspired material for the first wall. It will use carbon based materials since neutrons and hardradiations do not affect the state of carbon materials. The material should be thin enough so all neutrons and gamma rays will go through the material without damaging its structure. Candidate are fibers or mats of Carbon Nanotubes (CNT) or Graphene layers (GL).

An important function to be added to the material is the cooling of the wall. The molten salt FLiBe is at 640°C. The wall could be cooled by a fluid going through the CNT fibers or the Graphene layers by capillarity.

Capillarity effects inside a CNT material has been studied by several teams [2] but none has proved that a flow of CO2 could be created through the wall by only capillarity process. The analogy of trees pumping the water from the soil to the leaves is invocated here.

In order to create samples of wall materials, 3D nano-printing of CNT embedded into a nanoporous media will be performed. The capillarity parameters of the samples will be measured then the samples will undergo series of test in molten salt and under high neutronic flux to insure their durability in service. The final architecture will be then design following the tehnical requirements of the reactor.

Toward an "artificial tree" from the bio-inspiration of a sequoia tree We use nanotubes and nanofibers, for example, to facilitate the first wall cooling and CO_2 conversion, etc. Nanomaterials inspired by the "artificial tree" concept contain such properties as their thinness to pass much of the hard radiations with only lower energy photons to capture, their ability to pump and circulate liquid (water) without external pumps, etc.

Keywords: Carbon base materials, carbon nanotube, graphene layers, nano-3D printing, neutronics, fluorine salts, irradiation

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2. Void-Free Layered Polymeric Architectures via Capillary-Action of Nanoporous Films - Jeonyoon Lee, Seth S. Kessler, and Brian L. Wardle (MIT)
3. Fusion-driven Liquid Transmutator Operated Realtime by Laser T. Tajima1 , A. Necas , G. Mourou , S. Gales, and M. Leroy

Tuning the properties of 2D perovskites

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Abstract:

Hybrid organic-inorganic perovskites are very promising semiconductors for many optoelectronic applications. However, their use is limited by their poor stability under environmental conditions. Therefore, it is very important to tailor the properties of perovskites in order to improve their stability and to tune their photophysical properties at the same time.

In our work we investigated the excitonic features and stability properties of several synthetized 2D perovskites single crystals, obtained by changing the organic spacer. By increasing the hydrophobic nature of the organic spacer, we observed an improved material stability, thanks to the creation of a robust barrier that preserve the crystalline structure, hindering photo-degradation processes usually promoted by oxygen and moisture [1].

It is possible to further increase the stability of 2D perovskites by incorporating organic diammonium cations into inorganic framework, resulting in the formation of Dion Jacobson perovskites. In this way, we can replace weak van der Waals interaction between the inorganic layers with a strong hydrogen-bonding interaction, resulting in a class of perovskites with exceptional stability [2]. In addition, by changing the organic interlayer cation, is possible to tune their crystal structure, resulting in a different structural distortion, meaning as deviation of the corner sharing octahedral ($\widehat{PbIPb}$ angle) from the ideal value of 180°. This structural modulation leads to a photoluminescence blueshift, owed to a reduction of metal-halide overlap that will increase the band gap [3] (Figure 1). Our work introduces an easy method to engineer 2D perovskites achieving improved stability and tuning the excitonic features of these interesting hybrid semiconductors for next – generation of nanophotonic devices.

Keywords: 2D perovskites; Dion Jacobson; Ruddlesden Popper; single crystals; structural distortion; perovskite stability; photoluminescence.

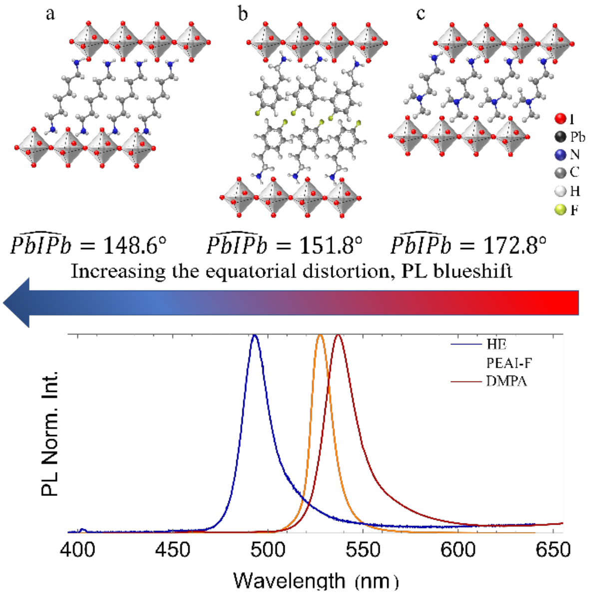

Figure 1: (Up) Crystal structure of the synthetized HE (a), PEAI-F (b) and DMPA (c) single crystals. (Bottom) Normalized photoluminescence spectra of synthetized perovskites. By increasing the equatorial distortion (decreasing the value of $\widehat{PbIPb}$ angle) there is a photoluminescence blueshift.

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Mott-insulator titanium sesquioxide: A novel electrochemical capacitor

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Abstract:
Novel electrochemical capacitance is observed in titanium sesquioxide (Ti_2O_3) a Mott-insulator with a narrow bandgap of ~ 0.1 eV. An anomalous increase in electrochemical capacitance is attained at the transition temperature after an ex-situ annealing of the material. Ti_2O_3-based planar solid-state (PVA/H_3PO_4) micro electrochemical capacitor showed an enhancement in areal capacitance (~560%) after annealing at 300 °C (ex-situ) as compared to the pristine Ti_2O_3 response. The transition from semiconducting to metallic states in Ti_2O_3 is attributed to the anomalous enhancement in capacitance. The total charge storage in Ti_2O_3 is quantitatively distinguished using Dunn's method, showing enhancement in electrical double-layer capacitance after annealing due to enhancement in charge density at the surface of Ti_2O_3. Further, density functional theoretical calculation (DFT) is performed for exhibiting the band merging ($E_g = 0$) after annealing at high temperatures. The increase in charge density of surface Ti atoms after annealing at high temperature is further supported using the Bader charge analysis and finding a good agreement with the electrochemical results. The high capacitance of 1053 $\mu F/cm^2$ is obtained with an aqueous electrolyte (1M H_3PO_4) and 307% enhancement in capacitance than the solid-state electrolyte.

Keywords: electrochemical capacitor, mott-insulator, titanium sesquioxide, solid-state, band merging.

Nanoparticles for High-Luminance Light-Emitting Diodes for Efficient Automotive Systems.

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Abstract:
The automotive industry is undergoing some technological and social revolutions that are shaping the greatest ever upheaval in transportation[1]. These forces are giving rise to three disruptive technological trends: electrification, autonomous vehicles, and digital mobility[2,3]. In the frame of these revolutions, nanotechnology is expected to play an important role. Specifically, quantum dots (QDs) might challenge the current lighting emitting diode (LED) and organic lighting emitting diode (OLED) technology used for customization and car-to-X communication as digital lighting devices for automotive systems. Thereby, we report a dynamic photoluminescence quantum dot light emitting device (QD-LED), with high luminance and uniformity characteristics (Figure 1). The QD-LED was designed with a quantum dot film (QDF) incorporating QDs tuned to 531 nm (green) and 624 nm (red) [4] . Thus, by exciting the QDF with 465 nm wavelength, it is possible to obtain white color light at the device output. By color-filtering that output all the automotive lighting functions (interior and exterior) could be performed. Moreover, state-of-the-art multichannel automotive LED drivers were used to allow the individual segment control, enabling therefore the digital communication with the vehicle surroundings[4]. That feature is used to share information to other road users through light, which is vital to support the autonomous vehicle development. Eventually, the low power consumption measured[4] implies a high electrical efficiency indicators, which is key to the carbon footprint reduction and the electrical vehicle transition, locating the use of this nanotechnology in an remarkable position in the next future of the vehicle transportation lighting systems.

Keywords: Nanotechnology, automotive lighting systems, electrical vehicle, autonomous vehicle, Quantum dots, QD-LED.

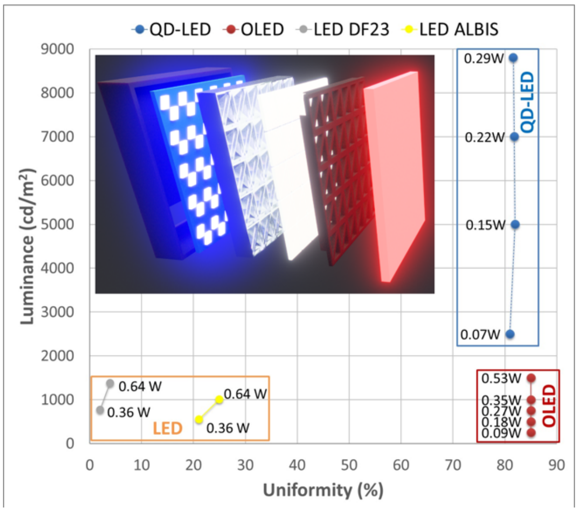

Figure 1: Figure illustrating the QD-LED designed[4], OLED and LED comparison of luminance vs uniformity values.

Acknowledgements
This work was supported by VALEO, multinational automotive company. F.M.G.C and S.R.B were supported by Project P18-RT-3303 funded by the Spanish Junta de Andalucía.

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Complementary reduced Graphene Oxide-based inverter for ion sensing

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Abstract:

Chemical Logic has been sparking much interest, as it provides a new and smart readout method and correlation of diagnosis thanks to Boole algebra. Graphene is an attractive material with high conductivity, stable in aqueous and biologic media and is therefore a great candidate for the fabrication of electronic devices in order to design chemical logic-based sensors.[1] Reduced Graphene Oxide-based (rGO) transistors offer competitive electrical performances suitable for low-voltage operations,[2] together with low-cost fabrication process, through surfactant-free graphene oxide inks directly deposited by inkjet printing methods, and further electrochemically *in-situ* reduced to obtain a conductive channel.[3] We investigate the design of inverters, in both complementary (transistors/transistors) and asymmetric (transistors/resistors) configuration from rGO Electrolyte Gated Field Effect Transistors (rGO-EGFET) able to provide a binary switch regarding the chemical signal applied at its input. In both cases, the inverter can be modelled by two variable resistors or one variable resistor and a fixed one, respectively in complementary configuration and asymmetric one. The output is then directly depending on the value of one resistor compared to the other one. In practice, as shown as a proof of concept (Figure 1), the switch from 1 to 0 occurs when the resistance of the first transistor (R_{T1}) becomes larger than that of the second (R_{T2}). The value of the resistance of each transistor is formerly tuned during the electrochemical reduction process, carried out by controlling the charge by chronocoulommetry.

Several applications, such as ion-sensors, are targeted for our graphene-based logic gates. In our case, the functionalization of one transistor's gate with molecules, binding specifically with targeted ions, is expected to shift the electrical properties of one transistor and provides the switch.

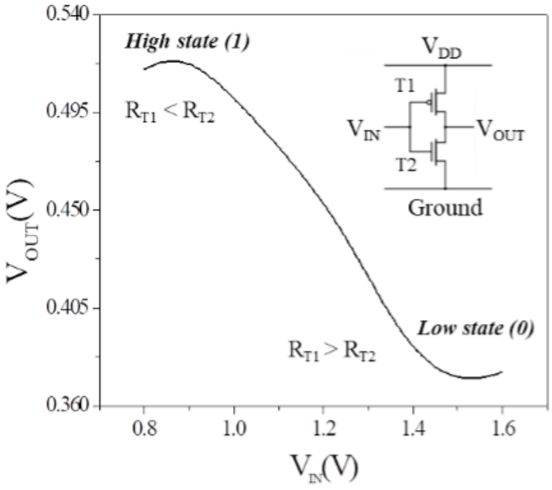

Figure 1: Input-output characteristic of a graphene-based inverter and its corresponding electrical model, for two GFET in different electrolytes: pure water (T1) and 0.5 M HCl (T2)

Keywords: Electrolyte-gated field-effect transistors, Chemical Logic, reduced graphene oxide-based inverters.

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Effect of 2D nanomaterials on MXene based engineered Aluminum plasmonic devices for bio-sensing in the near-infrared region

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Abstract:

In regard to surface plasmon excitation at the metal-dielectric interface, Aluminum (Al) has gained much attention in the recent past. Since it is cheaper as well as CMOS compatible, Al-based plasmonic devices are a popular choice for optoelectronic applications along with their ability to achieve better optical response in terms of narrow linewidth [1]. In order to functionalize the surface of the Al metal layer for biosensing applications, various 2D nanomaterials have been utilized [2]. Recently, MXene ($Ti_3C_2T_x$) has become a hot spot for sensitivity enhanced SPR sensors, due to its superior capacity for loading the biomolecules [3]. In this work, we have engineered Al-based plasmonic devices with MXene nanosheets to achieve both high sensitivity as well as Figure of Merit (FOM). The geometrical parameters for proposed plasmonic devices are optimized using Rigorous Coupled Wave Analysis for the wavelength of 1550 nm in the optical communication band. Since, studying 2D nanomaterials can provide quality collaboration for MXene, from their functionalization to application, fluorinated Graphene (Gr) and MoS_2 are undertaken for this purpose. The effect of such 2D nanomaterials has been studied on both sensitivity and FOM for Mexene based engineered Al-plasmonic sensor and a decent value of both sensitivity (139nm/RIU) as well as FOM (295.7RIU^{-1}) is achieved for a wavelength of 1550 nm in the Kretschmann's configuration. To demonstrate the bio-sensing application with the proposed plasmonic devices, the detection for the SARS-COV2 virus, based on the change in their refractive indices, is carried out. The proposed MXene based Al-plasmonic devices show promising applications in the optical communication band, employing Gr and MoS_2 in the NIR region.

Keywords: Surface Plasmon, Aluminum, Mxene, SPR sensors, NIR region, Sensitivity, Figure of Merit

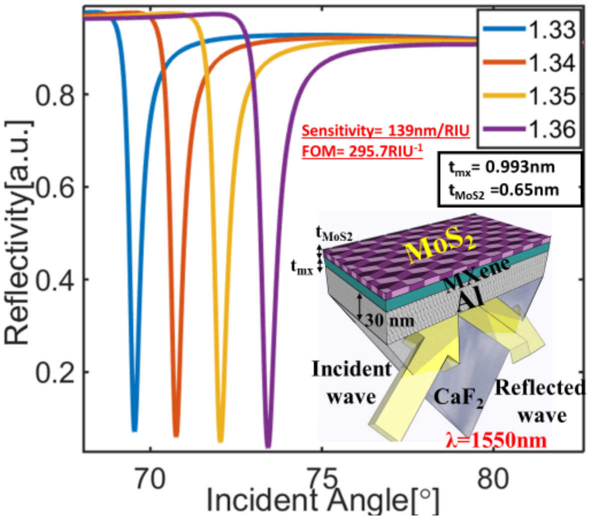

Figure 1: Reflectivity curves with the variation in the refractive index of analyte for proposed Mexene based Al-plasmonic devices for a wavelength of 1550nm (schematically shown in the inset)

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An Unified Approach for Nanoplasmonics of Metal and Graphene-Based Nanostructures

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Abstract:

Most properties of plasmonic nanostructures follow from the tunability of their optical response as a function of their shape and dimensions [1]. Such a feature is typical not only of metal nanoparticles but also graphene-based nanostructures, for which an additional tunability, based on electrical gating, can be exploited. The accurate description of the optical properties of the plasmonic substrates is crucial for a theoretical understanding of the physical phenomena occurring at the plasmon resonance frequency [2]. Here, we present an atomistic, yet classical, approach to predict the plasmon properties of nanostructures of complex shapes. Our approach is general enough to describe, at the same time and with the same level of accuracy, metal nanoparticles [3,4] and graphene-based nanoaggregates [5], being able to correctly reproduce the experimental trends.

Besides the potentialities of our approach for large scale nanoplasmonic simulations, we also show that a classical approach, in which the atomistic discretization of matter is properly accounted for, can accurately describe the nanoplasmonics of systems dominated by quantum effects, such as subnanometer junctions [3,6] or by geometrical defects, as for polycrystalline graphene. In particular, in the selected test cases we will show how to engineer matter at the nanoscale to create very localized hot-spots, with potential application to single molecule detection [6,7].

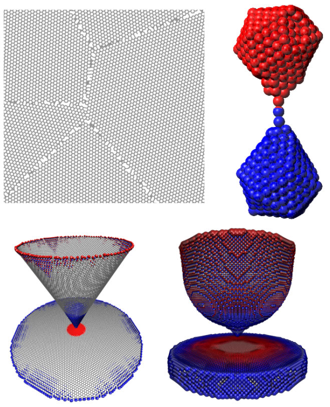

Figure 1: Different examples of the systems that can be investigated by exploiting our approach: a polycrystalline graphene sheet (top left), a subnanometer junction (top right), and two hot-spots created in a graphene-based (bottom left) and a metal (bottom right) nanoaggregates.

Keywords: Metal Nanoparticles, Graphene, Nanoaggregates, Modeling, Atomistic simulation, plasmonics, quantum tunneling, subnanometer junctions.

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Acknowlegment

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Two-dimensionnal substrate (MXene, graphene) supported nickel/iron-based catalysts for oxygen evolution reaction in alkaline medium

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Abstract:
Water splitting is a process providing an interesting pathway to convert intermittent renewable energies into hydrogen, a chemical fuel possessing a very large specific energy density (ca. 33 000 Wh kg^{-1}). Performances of water electrolyzers are currently hampered by the sluggish kinetics of oxygen evolution reaction. While only Ru-and/or Ir based catalysts have demonstrated a huge OER activity in acidic solutions, a number of nonprecious metal oxides are reported to have a high activity in alkaline solutions. Among all these catalysts, nickel and iron based materials are currently the most promising ones.

Here, we describe two-dimensionnal substrate (MXene, heteroatom doped reduced graphene oxide) supported nickel-iron based catalysts that exhibit a very high OER activity in alkaline solutions (**Figure 1**). Two different families have been investigated, that is to know NiFe nanoparticles deposited onto Mo_2CT_x MXene (where T is the terminal group: -OH, F, and/or -O) and nickel/iron sulfide nanoparticles supported onto N,S doped reduced graphene oxide. These materials are respectively easily synthesized using a one-pot solvothermal method or a wet impregnation procedure followed by a heat-treatment. Fisrt, it was demonstrated that the presence of the two-dimensionnal substrate allows modifying phase selectivity during the synthesis. Secondly, under electrochemical conditions (potential cycling) synthesized materials were demonstrated to be subjected to surface restructuring phenomenon. Phases formed at the surface of nanoparticles subsequently to surface reconstruction allows greatly improving OER activity in alkaline medium. Furthermore stability tests under galvanostatic conditions (current density of 10 mA cm^{-2}geo, 8 M KOH electrolyte) were performed and these catalysts were stable for more than 400 hours.

During this presentation the morphology, structure, composition and catalytic properties of materials will be discussed on the basis of results obtained from classical physico-chemical characterization techniques (XRD, TEM, XPS) and electrochemical methods (cyclic voltammetry, electrochemical impedance spectroscopy). A special attention will be carried out to the in situ characterization of surface restructuring phenomenon in order to understand the entanglement between the properties of the reconstructed catalytic surface and its OER activity.

Keywords: MXene, graphene, electrocatalysis, oxygen evolution reaction

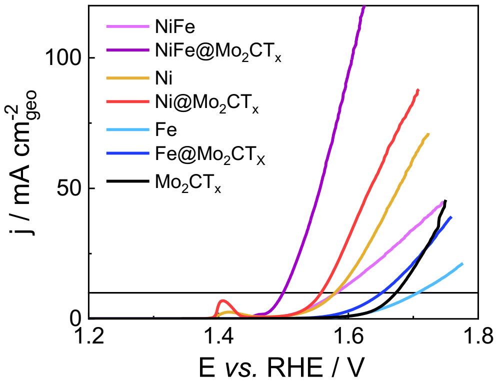

Figure 1: Polarization curves registered after 100 voltammetric cycles between 0.5 and 1.5 V vs. RHE. Experiments were done in a N_2 saturated KOH electrolyte (1 M) using NiFe nanoparticles deposited onto Mo_2CT_x MXene. Scan rate 5 mV s^{-1}.

Synthesis and Modeling of Supported Bimetallic Iron- and Copper Oxide nanoparticles and their Application in Fenton Reaction

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Abstract:

In the Fenton reaction, metal (oxide) based catalysts are used to convert hydrogen peroxide into hydroxyl radicals, which, subsequently, degrade organic pollutants in aqueous solutions. Bimetallic combinations of nanoparticles, such as iron-oxide/copper-oxide, have shown synergistic effects in this reaction, reaching much higher hydrogen peroxide conversion rates than their monometallic counterparts. For the synthesis of these bimetallic catalysts, impregnation synthesis is a cheap and scalable method.

Impregnation based synthesis is one of the most commonly used synthesis methods for preparing supported nanoparticles, both in industry and research. Recent research, however, has shown that final catalyst properties can be very sensitive to the synthesis conditions applied during the impregnation step[1]. Parameters such as the pH of the impregnation solution, the concentration and type of counter-ions present, and the surface properties of the support material will impact the interactions taking placing between the dissolved metal species and support surface during impregnation. These interactions can alter both the microscopic properties (nanoparticle size and shape) and macroscopic properties (distribution of the metal throughout the support material) of the final material. During the synthesis of bimetallic materials, these interactions are further complicated by the presence of the second metal, which can either be impregnated simultaneously with the first metal, or in a separate impregnation step.

In this work, the effects of the above mentioned synthesis conditions on the macroscopic and microscopic properties of Fe_2O_3/CuO nanoparticles supported on Al_2O_3 microspheres, prepared both by simultaneous and sequential impregnation of the metals, are studied. The interactions taking place during impregnation are modelled, in order to clarify the mechanisms by which the observed variations in material properties are formed. The synthesized materials are then used as catalysts for the Fenton degradation of methyl orange, to reveal which material properties are key contributors to the catalysis and synergy between the two metal oxides.

Keywords: Synthesis, Modelling, Heterogeneous Catalysis, Nanoparticles, Hybrid materials

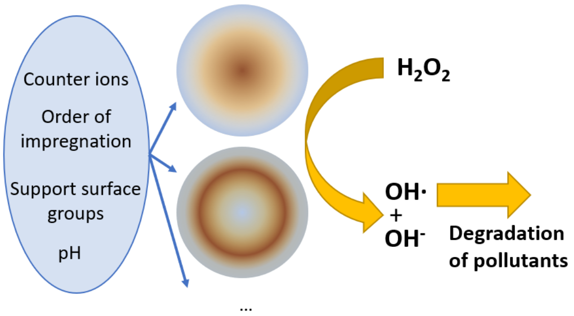

Figure 1: Schematic illustration of the synthesis of supported bimetallic iron- and copper oxide catalysts under varying synthesis conditions (left), and their application in producing hydroxyl radicals for the degradation of pollutants (right).

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Controlled loading of single atoms in oxygen vacancies as a co-catalyst on TiO_{2-x} nanotube reduced by ultrasonication

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Abstract:

Single-atom catalysts (SACs) due to utmost atom efficiency, propose great potential to show high selectivity and excellent catalytic behavior in variety of chemical reactions compared to nanoparticles catalysts (NPCs). In this work, an innovative method to stabilize Pt single-atomic site by constructing atomic-scale defects on the surface of TiO_2 nanotubes arrays for photocatalytic H_2 evolution is presented. Highly-ordered TiO_2 nanotubes (TNTs) have been synthesized on the Ti foil using a simple electrochemical anodization method. To form single-atomic site Pt supported on defective TNTs, tip sonication machine was employed, followed by soaking the substrate in very dilute hexachloroplatinic acid solution. As a proof of this concept, by a combination of HRXPS, HRTEM, UV-DRS, density of state (DOS) and Mott-Schottky plots to the TNTs film, Pt in atomic scale can be confirmed. The optimized Pt single-atom (Pt-SA) catalyst showed an excellent performance for hydrogen evolution in 1 sun solar light (AM 1.5-100 mW/cm^2) such that the large normalized hydrogen evolution yield was more than 900 percent higher than that produce by Pt nanoparticles (Pt-NP) decorate sample. Therefore, it is believed that this study paves a new way to construct highly active single atomic site catalysts on oxide supports layer.

Keywords: TiO_2 nanotubes (TNTs), Platinum (Pt), Single-atom catalysts (SACs), H_2 evolution, PEC activity

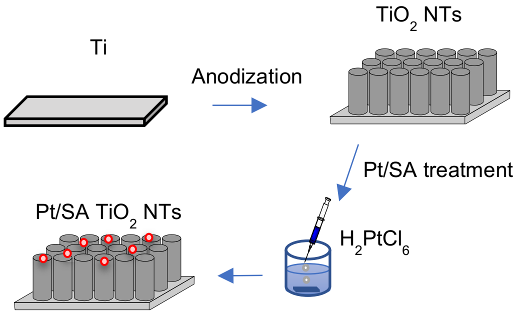

Figure 1: Schematic illustration of preparation Pt/SA TiO_2 NTs.

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Ternary phosphides (Cu_xCo_yP) as efficient electrocataysts for HER and OER

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Abstract:
Transition metal phosphides are appealing materials to be used as affordable and efficient catalysts in several processes including hydro-processing, water-gas-shift reaction, HER, OER and for overall water splitting. Specifically, copper based nanocatalysts are widely used as catalysts for various reactions because of their wide range of accessible copper oxidation states and high melting point. Recent reports found that ternary phosphides have better catalytic activity and selectivity towards the oxygen reduction reaction (OER) and alcohol oxidation than the binary materials. Herein, we report the synthesis, characterization and the study of the catalytic properties of copper phosphide nanoparticles and their ternary derivatives with Co. We do so to explore the effect of alloying Co in copper phosphide system and how it affects the morphology, stability and catalytic activity as cobalt phosphide nanoparticles have been proved to be quite stable and good catalysts for HER, OER etc. In alkaline media (1M KOH) the best catalysts in the sample set was $(Cu_{50}Co_{50})_3P$ which exhibited an overpotential of 184mV at 10 mA cm^{-2}. In addition, $(Cu_xCo_y)_3P$ were active OER and methanol oxidation catalysts in alkaline media (1 M KOH). The best catalyst in the sample set for OER was $(Cu_{25}Co_{75})_3P$ which showed an overpotential of 283 mV at 10 mA cm^{-2}. This study not only provides information about new strategy of synthesizing ternary compounds of earth abundant metal phosphides but also gives insights about synergistic effect of Cu with Co in a phosphide system, which can be a promising cathode material for overall water splitting and alternative energy resource in future application.

Keywords: Ternary metal phosphides, Nanocatalysts, Electrocatalysts, Hydrogen evolution reaction (HER), Oxygen evolution reaction (OER), Overpotential.

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Nanotech / GAMS 2022
Joint Session II.B:
Nanocoatings/ Thin films and nanostructured surfaces

A comparative study between blended polymers and copolymers as emitting films for single-layer white OLEDs

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Abstract:
White organic light emitting diodes (WOLEDs), processed from solution, have attracted significant research interest in recent years due to their superior advantages such as low device production cost, device flexibility, easy fabrication over large area including roll-to-roll and ability to print in various designs and shapes providing enormous design possibilities especially for lighting applications. WOLEDs with a single emissive layer, either using fluorescent or phosphorescent dopants in a host material, or copolymers that bearing different chromophores have been proposed as promising methodologies for the easy fabrication of high-performance devices as they are alternatives of the complicated multilayer device architectures using expensive emissive materials and more fabrication steps. However, precise control of the dopant concentration in the guest−host system, for the case of blends, or of the chromophore ratio, for the case of copolymers, are essential for achieving the required color coordinates. Thus, despite the multifaceted efforts, the successful market penetration of OLED-based lighting products is still elusive because of the high fabrication costs, material costs, and stability issues. In this work, were utilized commercial blue Poly(9,9-di-n-octylfluorenyl-2,7-diyl) (PFO), green Poly(9,9-dioctylfluorene-alt-benzothiadiazole) (F8BT) and red spiro-copolymer (SPR) light-emitting materials to develop blends, and Distyrylanthracene, distyrylcarbazole and distyrylbenzothiadiazole chromophores as yellow, blue and orange-red emitters, respectively, to synthesize novel copolymers. Single layer WOLED devices of two- and three-phase blends and copolymers bearing two and three chromophores were fabricated either by spin coating or slot-die processes. The produced films and devices were characterized in terms of their optical and photophysical properties using Spectroscopic Ellipsometry and Photoluminescence Spectroscopy, accordingly, of their surface nanotopography using Atomic Force Microscopy and of their electrooptical properties using Electroluminescence Spectroscopy.

Keywords: WOLED, PFO, F8BT, anthracene, carbazole, benzothiadiazole, blends, copolymers, spin coating, slot-die, ellipsometry, photoluminescence, electroluminescence, photophysical properties, electrooptical properties, lighting applications.

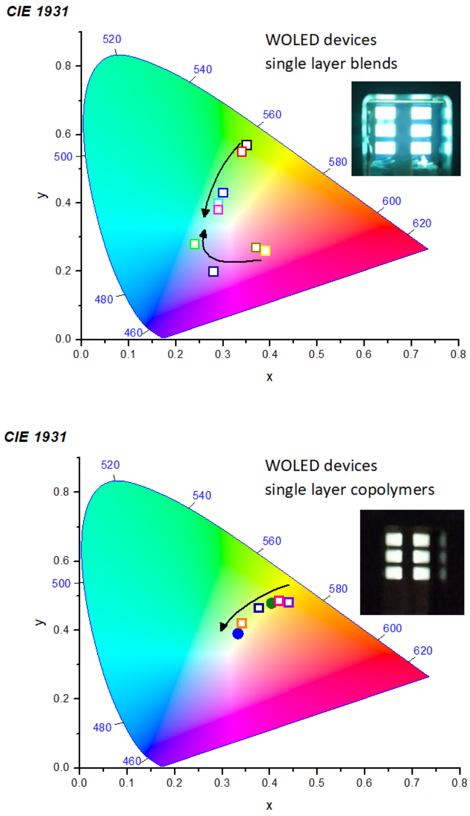

Figure 1: The EL CIE color coordinates of the OLED devices with single layer blends and copolymers.

Acknowledgements: This research has been co-funded by the European Regional Development Fund of the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship, and Innovation, under the call RESEARCH—CREATE—INNOVATE (project code: T1EDK-01039).

The influence of the nano-structured architecture type on the optical, electrical and thermal properties of TiN coatings

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Abstract:

Titanium nitride (TiN) coatings have been and are widely used in practice, especially for improving the mechanical and tribological properties of contact surfaces.

TiN coatings have outstanding characteristics such as high hardness, low friction coefficient, good wear and oxidation resistance, which can be maintained even in reatively high temperature conditions.

Although the tribological coatings of Me-N type (Me – transition metal such us: Ti, V, Cr, Ta…) have been very much studied, for different processes and deposition conditions, lately, the researchers' attention has been shifted to the possibility to change their structural architecture, namely in what concerns to the improvement of their exploitation properties. In this sense, the present work is focused on the analysis of two important variables: the characterization of nanostructured-like coatings and the tailoring of their properties by using a zig-zag-like growing architecture.

To carry out this, TiN coatings have been deposited on spring-steel and silicon substrates, by DC reactive magnetron sputtering, by varying the power discharge. The deposition process consists of a confocal configuration of two magnetrons (with two Ti targets) with a substrate holder placed at the top-central position inside the reactor, Fig. 1. Two sets of samples with different architectural aspects have been obtained. The first set involved the use of both magnetrons simultaneously, with the substrate samples rotating continuously during the deposition process – conventional prowth samples. The second one consist on the use of the magnetrons alternately, keeping the samples in a fixed position, in order to obtain a special zig-zag-like architecture.

Both architectural variants have been investigated in terms of morphology, structure and deposition rates. At the same time mechanical and tribological properties are studied and correlated with the deposition parameters and the micro(structural) features in order to compare the performances of the two architecture variants. Moreover, the influence of the power discharge on the final properties of the coatings has been investigated.

Keywords: TiN films, coatings, zig-zag structure, tribological properties, mechanical properties.

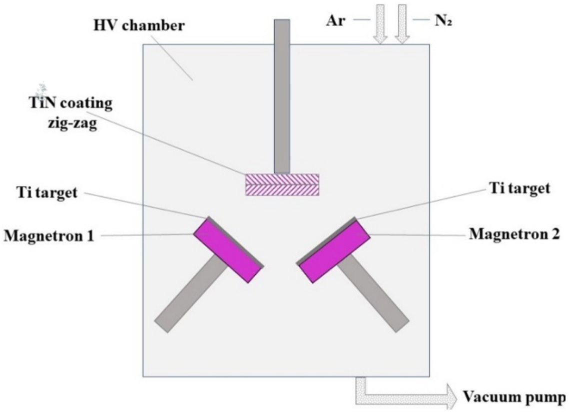

Figure 1: Figure illustrating the system through which the zig-zag structure of TiN films is obtained.

Dielectric Properties of $Ca_3Mn_2O_7$ thin films prepared by Pulsed Laser Deposition

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Abstract:

Naturally Layered Perovskite structures with improper ferroelectricity [1, 2], such as the Ruddlesden-Popper calcium manganite compound $Ca_3Mn_2O_7$, offer an alternative route to achieve non-expensive and high-performance room temperature multiferroic magnetoelectricity for information storage, sensors, and actuators or low power energy-efficient electronics. They allow exploring oxygen octahedra nonpolar rotations and cation site displacement to attain non-centrosymmetry. Additionally, due to their high sensitivity to lattice-distortions, their preparation in thin film form over crystalline substrates allows the manipulation of acentricity and enables the tuning of lattice, electric and magnetic interactions. As such, thin films of $Ca_3Mn_2O_7$ have been prepared over $SrTiO_3$ substrates by Pulsed Laser Deposition, using a $Ca_3Mn_2O_7$ target. The structural studies show that in the films prepared on $SrTiO_3$, at 730 ºC, with 4 J/cm^2 laser fluence, 10^{-3} mbar oxygen pressure and with a post-annealing process, the $Ca_2Mn_3O_7$ phase is stabilized, as confirmed by EDS, XRD and Raman Spectroscopy. The $A2_1am$ ferroelectric phase was observed to be present in the films, along with the orthorhombic Acaa, phase, with a preferential (111) growth direction and substrate-induced enhancement of the polar ferroelectric distortion. The dielectric permittivity of the films shows the presence of dispersion described by the Havriliak-Negami model function with two relaxations. From temperature-dependent fits to the permittivity curves, a different behaviour of the parameters was observed above and below the antiferromagnetic phase transition. Additionally, the Kohlrausch-Williams-Watts stretched exponential parameter showed an abrupt decrease below ~112 K (Figure 1), near the Neel temperature, indicating magnetically induced enhancement of dipolar-correlations with decreasing temperature. The structural and dielectric properties of the films will be discussed and presented, highlighting the polar cooperative behavior and phase evolution and stabilization in the films.

Keywords: Naturally Layered Perovskites, Ruddlesden-Popper, Calcium manganese oxide, Thin films, Pulsed Laser Deposition, Structural Properties, Dielectric Properties

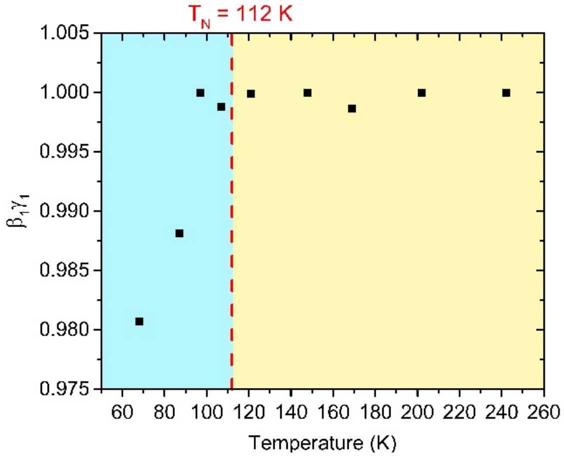

Figure 1: Temperature dependence of the stretched exponential parameter, β_{KWW} marked with an abrupt decrease of observed bellow ~112 K.

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Reactivity at the interface between metals and Bi_2Se_3 topological insulator.

M. Fanetti [1,*], K. Ferfolja [1], S. Gardonio[1], M. Valant[1]

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Abstract:

The interfaces between metals and topological insulators (TIs) are present almost everywhere when TIs are used in prototypes and applications, from catalysis to spintronics, down to the fabrication of simple electric contacts. The interface structure is of crucial importance, since the special properties of TIs reside in the topological electronic states at the surface. However, such interface is far from being a simple connection between the metal and the TI crystal.

In our study we analyzed Bi_2Se_3 – one of the most studied TI – interfaced with four different metals: Au, Pt, Ag and Ti. Their application span from electric contacts (Au, Ti) to catalysis (Pt) and spintronics (Ag). These interfaces have been deeply characterized by means of a variety of techniques, such as electron microscopy (TEM, SEM coupled with in-situ heating), energy dispersive X-ray spectroscopy (EDX), X-ray photoemission spectroscopy (XPS), and others.

With the only exception of Au/Bi_2Se_3 (Figure 1, top), where only a weak interaction without the formation of an interfacial phase has been detected, in the other cases a chemical instability has been observed at the interfaces, with the occurrence of chemical reactions and formation of new phases. In the case of Ag the solid state redox reaction occurs at room temperature, with observable migration of Ag atoms within the Bi_2Se_3 crystal. With Ti (Figure 1, bottom) a chemical reaction is detected even at cryogenic temperature (130 K), with formation of $TiSe_2$.

Our results are combined with previously published studies to highlight the general trends of the behavior of metals when interfaced with Bi_2Se_3 and to explain its unexpected reactivity.

The exposed results are of fundamental importance for the exploitation of TIs properties, and have to be taken into account when designing a TI based system for applications.

Keywords: topological insulators, thin films, metal/TI interfaces, topological surface states, solid-state reaction

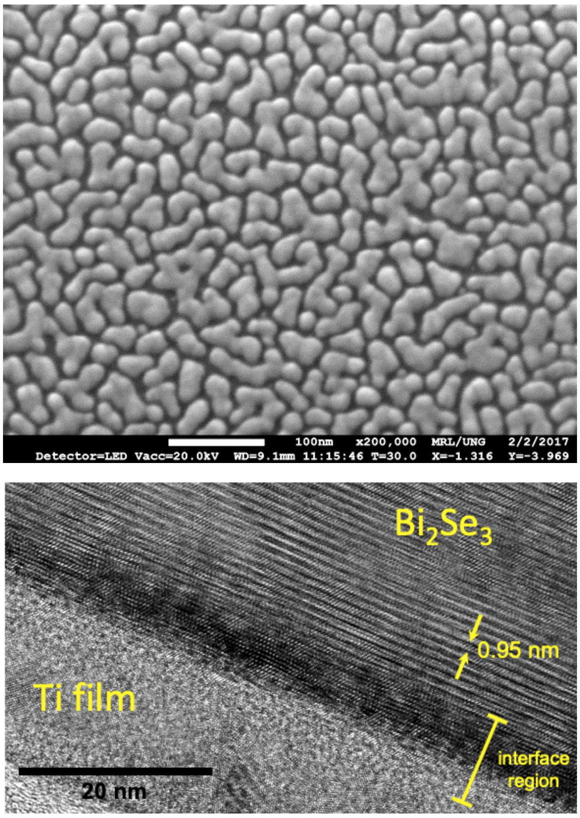

Figure 1: (top) SEM image of Au thin film (10 nm) deposited on Bi_2Se_3 (0001) surface. (bottom) TEM image (X-section) of Ti thin film (20 nm) deposited on Bi_2Se_3 (0001) surface.

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Low Velocity Impact Behaviour of Composite Laminates Containing TiC and ZrC Nano-Particles in Resin System

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Abstract:

Composite structures utilized in defence and aerospace applications might be subjected to impacts due to bird strike, tool dropping and bullet penetration. Therefore, low velocity impacts have to be considered when designing and manufacturing of composites. This encouraged people to create and analyse tougher and stiffer composite materials in recent years. One of the approaches to this problem is to add nano tubes and nano particles to resin systems in order to improve bonding between fibres and matrix materials. Different nano-particles or nano-tubes of clays, alumina, silica, carbon and graphene have been analysed in composite systems in the literature so far because of the improved mechanical properties.

In this study, the low velocity impact behaviour of the aramid fibre reinforced epoxy composite plates, containing two new nano-particles of TiC and ZrC which are not studied formerly, are searched experimentally. For this, nano-particle free, ZrC and TiC nano-particle containing composite plates were produced with hand lay-up method in a way to obtain an orientation as 7 layers of aramid fibre fabric reinforced epoxy resin containing nano-particles, $[0°/45]_7$. Then, the behaviour of the composite plates against low velocity impact by means of an impactor dropped from a fixed height with a fixed potential energy were studied. The contribution of TiC and ZrC nano-particle additive to impact resistance have been explained by means of the load-time, energy-time and displacement-time. After the low velocity impact tests, it is concluded that plates containing titanium carbide nano-particles yielded 19 % less penetration in comparison with particle free plates. In other words, it showed more resistance against the impact by 19 % against to particle free plates. On the other hand, although plates containing zirconium nano-particles are more resistant to low velocity impacts in comparison with particle free plates by 4 %, it has been determined that its contribution in terms of impact resistance remained lower than the plates containing titanium nano-particles

Keywords: Low velocity impact, nano-particles, ZiC, TiC, aramid composite plates

Table 1: Table shows there is a good correlation between penetration depth (total displacement) and maximum impacting force. Higher impacting force measured means lower penetration depth.

Sample	Max Energy [Joule]	Peak Load [N]	Penetration (dent) depth [mm]	Penetration Improvement [%]	Thickness [mm]
Control (plain)	40,754	4799,7	6,318	-	2,7675
TiC Modified	41,242	6020,0	5,104	19	3,0708
ZrC Modified	42,122	5380,8	6,079	4	3,1114

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Kinetically Controlled On-Surface Playground of Nanostructure Growth

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Abstract

Rare gases on metals serve as models for understanding adsorption, mass transport and crystal growth of adsorbates on surfaces, while LT-STM studies enriched our knowledge how rare gases behave at atomic level. Unprecedented insight has been gained into the diffusion mechanisms of van der Waals adsorbates on a complex energy landscape defined by an on-surface coordination network architecture. Using Xe as the model case, a complex re-distribution/re-nucleation and coarsening/growth phenomena has been investigated where the adsorbate can be evaporated/re-captured into/from 'gas phases' or 'lattice gas phases'. The participation of different thermodynamic reservoirs to host diffusing Xe is observed to be changing in many steps between 5K and 50K. While only very few Xe atoms are already mobile at 5K after surface adsorption hopping motion between different confinements (0D) and then also along the boundaries of the network (1D) and across the whole network backbone (2D) becomes thermally activated. This gradual activation of different reservoirs for thermodynamically activated diffusion also leads to gradual re-equilibration of Xe atoms which are originally confined in more Energy minimal states of the complex surface potential . After heating to ~50K and cooling back to 5K the Xe atoms are almost exclusively found in the thermally minimal state of 12 Xe atoms filling one pore, a process which we assing to the analogon of Ostwald ripening and coarsening transition which is in the case of these nanometer confined porous network clearly limited in size. By the capability to design on-surface architectures complex functions may be realizable, far beyond the demonstrated capability to adsorb 12 Xe atoms per pore. It may be envisioned that the specific environment of a pore containing specific electronic states is not only a capable absorber, but also a very specific catalytic reaction environment that can be loaded/unloaded via the diffusion mechanisms, in the specific case for trapping atoms or molecules.

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Core-shell nanofibers as coating re-inforcement

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Abstract:
In the present approach the performance coating re-inforced electrospun core-shell nanofibers towards various functionalities was evaluated. Electrospinning is a well-established and flexible process which already demonstrated the manufacturing up-scale mass production capability with relatively low costs. Continuous, ultrafine fibres with uniform morphology, high surface area, high surface roughness and low weight can be generated.

Optimization of the electrospinning parameters was done to achieve the formation of beads free nanostructures. Core-shell nanofibers were incorporated into a commercially available paint. Nanostructured materials were placed either directly on the aluminium substrate, either in a sandwiched structure, in between two coating layers with different thicknesses. Scanning electron microscopy (SEM) was used to investigate the morphology of the core-shell nanofibers. Their layer thickness, as measured by focused ion beam (FIB), was tailored between 1 and 50 µm. Surface wettability was investigated by means of contact angel measurements. Furthermore, water contact angle performed at various temperature (from room temperaturute until -20°C) pointing out the potencialof the these untionalised coating in delaying ice formation. Adhesion of the commercially available coating with and without core-shell nanostructures was measured by performing cross cuts test according to ISO 2409. Coating resistance was investigated by immersion in various solution with the pH ranging from 1 to 13, immersion time vas tailored between 1 to 24 hours. Additionally, electrochemical impedance spectroscopy (EIS) measurements were performed to characterize the effect of incorporating the core-shell nanofibers into the coatings and to evaluate their performance in protecting aluminium against corrosion.

Keywords: coatings, core-shell nanofibers, corrosion, anti-icing

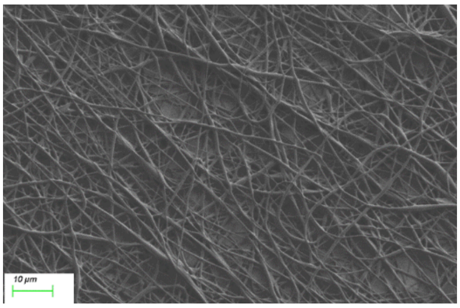

Figure 1: SEM image of core-shell nanofibers

Intelligent coating systems on multimetallic composite structures for automotive production

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Abstract:

The application of light weight metals in automotive structures reduces the weight of the vehicles and therefore their fuel consumption. This helps to reduce CO_2 emission and to reach the EU-targets regarding climate protection. One approach towards implementation of lightweight structures is the substitution of multi-component steel parts by single component die cast parts. A further approach, which combines multiple aspects of lightweight construction is the application of multi-material-design – combining components of high-strength steel, Aluminium and Magnesium alloys and carbon fibre reinforced plastics (CFRP)s [1]. CAR estimates, that 96% of all automotive programmes will consider the application of Aluminium as construction material for car bodies until the year 2030. Besides aluminium, Magnesium becomes more and more important, as its application will further reduce the weight of cars. The amount of aluminium in an average car has increased from 50 kg in 1990 to today’s 151 kg. Experts projects that this could rise to 196 kg by 2025. Aluminium in cars is already an excellent example of a circular economy. More than 90% of the metal is recovered after the end of the vehicle’s life-cycle and reused to create new aluminium products [2].

The biggest challenge concerning the application of lightweight metals is galvanic corrosion (contact corrosion), which occurs, when dissimilar metals (with dissimilar electrochemical potentials) are in electrically conductive contact with each other in presence of an electrolyte. To counteract corrosion (including contact corrosion), measures for corrosion protection are required. In automotive industry, corrosion protection is usually applied after assembly of the car body (and other parts of the car), by chemical pre-treatment – (degreasing; passivation by phosphating or zirconium oxide process) – and electrophoretic (usually cataphoretic) dip-coating, followed by application of a layer system of sealing, base coat and top coat [3]. As of now, there is no pre-treatment process available, which would be compatible with Magnesium alloys in assembly with (galvanized) steel and/or aluminium alloys. Therefore, Magnesium coatings must be subjected to a cost-intensive off-line pre-coating before assembly. This circumstance hinders the broad application of Mg alloys in automotive Industry - as of now, the use of Magnesium parts is more or less limited to upper class, luxury- and sports cars, and only slowly penetrates into middle class cars of higher-priced brands.

Within the framework of the IBM-Sys project (2021-2022, 80% financed by FFG Austria,project 884352 in “MdZ 15”), our objectives are to develop and test novel pre-treatment processes for the pre-treatment of steel, aluminium and magnesium assemblies prior to electrophoretic dip coating without the need for off-line treatment or coating of the magnesium components. The preliminary results will be presented and discussed in this study. The requirements for coating systems for multi-material composites and the possible solutions to be investigated will bring new insights into the research and development of coating systems.

Keywords: light weight structures / CO_2 emission reduction, multi-material-design, galvanic corrosion, corrosion protection, layers systems, automobil applications (car body).

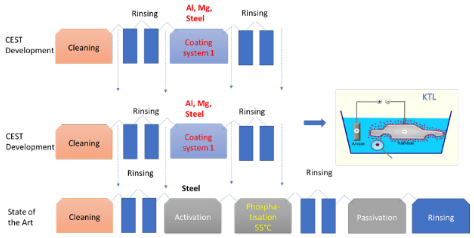

Figure 1: Figure illustrating CEST Coating systems on multi-metal assemblies with aluminium, magnesium, and steel components / Comparison State of the Art (steel).

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3. Automotive Paints and Coatings. Edited by H.-J. Streitberger and K.-F. Dossel ¨ Copyright 2008 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim ISBN: 978-3-527-30971-9

Correlation microstructure-heat treatments-mechanical properties of stainless steel 316L parts obtained by additive manufacturing

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Abstract:

Metal additive manufacturing, and more specifically Selective Laser Melting (SLM), is an ideal means to obtain parts with complex geometries impossible with so-called conventional manufacturing methods (wrought, casting, rolling, etc.). Among the most commonly used families of alloys, we find the family of steels. Within the family of steels, the AISI 316L grade is widely used because of its numerous industrial applications in several sectors: medical, aeronautical, automobile, petroleum, etc. 316L stainless steel is mainly used for its resistance to corrosion in highly corrosive environments and its mechanical properties at high temperatures. SLM induces a microstructure consisting of columnar grains with a dendritic substructure composed of dislocation cells [1]. This microstructure is different from conventional 316L steel (with equiaxed and twinned grains) and is due to a very high cooling rate of the molten metal (of the order of 10^6-10^8 k/s). On the other hand, this technology generates significant heterogeneities within the parts, which can be detrimental to the mechanical properties of parts in service. This heterogeneity linked to the manufacturing process is due to a different thermal history within the parts throughout the manufacturing process [2]. The geometries of the parts are complex but their usage properties are degraded. The objective of this work is to bring our 316L obtained by SLM to mechanical properties close to those of conventional 316L steel while taking advantage of the geometrical possibilities of shaping the parts offered by additive manufacturing. To achieve this, a series of heat treatments were carried out. In particular, a first solution heat treatment with quenching was carried out in order to homogenize the material and obtain a microstructure and mechanical properties close to those of 316L steel. Then second heat treatments of tempering at different temperatures were carried out in order to bring our material to different ranges of mechanical properties. In our report, we will discuss the influence of heat treatments on the mechanical properties and the impact of these heat treatments on the corrosion resistance of 316L parts. A correlation between the microstructure and the characteristics of the passivation layer will feed our discussion. We will also discuss the influence of the manufacturing process (SLM vs. conventional) on these two characteristics by comparing the results of mechanical tests (traction, hardness) and electrochemical corrosion tests in a chlorinated medium.

Keywords: Additive manufacturing, SLM, stainless steel, AISI 316L, annealing treatment, tempering treatment, corrosion, mechanical properties.

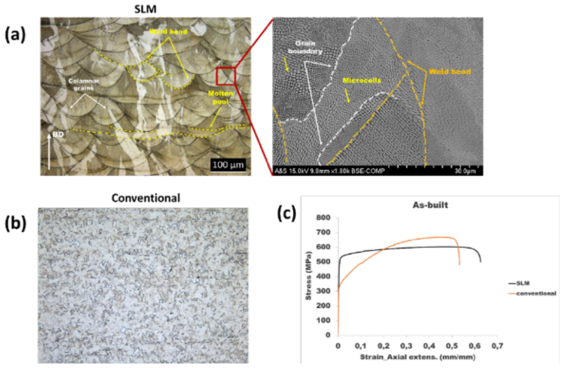

Figure 1: figure illustrating the microstructures of 316L-SLM (a), 316L-conventional (b) and the difference in mechanical properties between these two materials as shown by their tensile curves.

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An interaction study of epoxy varnishes with different metal oxides

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Abstract:
Bonding of metal surfaces with adhesives is dependent on base-acid interactions between the coating and the metal surface. The chemical structure and morphology of the metal oxide passivation layer has an important impact on these interactions. Hence, sheets of pure Zn, Sn and Al were investigated in the uncoated reference state and characterized by X-ray photoelectron spectroscopy (XPS). Furthermore, components of the water-borne model epoxy varnish and the epoxy coating on the metal substrates were also analysed by XPS.
To model a possible reaction between the used hardener dicyandiamide (DICY) and the metal oxides, the substrates were immersed in a solution of DICY in pure water. By XPS analysis chemical reactions of the amine groups of DICY with the metal oxides were ascertained. Performing cryo ultra-low-angle microtomy (cryo-ULAM), a preparation technique which has proven to be successful for depth profiling of polymeric samples without destroying the chemistry, it was confirmed that a similar reaction occurs even in the more complex system of the model epoxy coating and the metal oxide passivation layer. Moreover, an enrichment of DICY hardener at the metal/polymer interface was detected for Zn and Sn substrates.

Keywords: Adhesive, metal/polymer interface, XPS, cryo ultra-low-angle microtomy

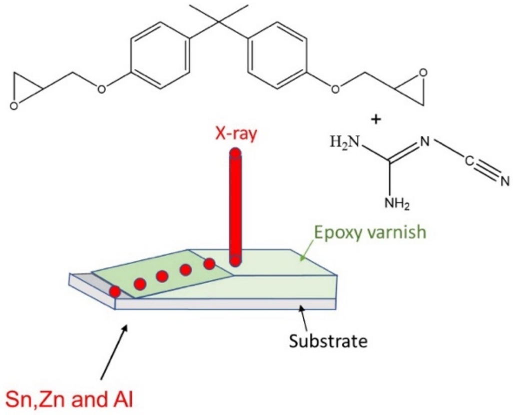

Figure 1: By preparing extended tapers with cryo-ULAM different depths of epoxy coatings on metal substrates could be investigated by XPS. A change of the chemistry of the coating near to the metal/polymer interface was detected, due to an interaction of the amine groups of the hardener DICY and the metal oxides.

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Au nanoparticles coated Au/Ag mirror as SERS active substrate for trace chemical detection

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Abstract:

In this work, we have presented a design of sensitive and easy to fabricate SERS substrate constituting of chemically synthesized Au nanoparticles (Figure 2) of varying sizes (radius=10-40nm); drop-casted on SiO2 (coverslip, thickness~170 um) whose bottom surface is coated (using thermal evaporation) with a uniform, thin layer of Ag/Au (thickness~50nm). The laser source with λ=785nm is irradiated on the substrate on which the sample to be identified/analysed is drop-casted, here we have used Rhodamine 6G (R6G) (sigma Aldrich) as probe molecule. The Au NPs gives rise to excitation of SPP, thereby ensuring electromagnetic enhancement. The thin Ag/Au layer at the bottom, produces a reflected wave which upon interaction with NPs from below, produces further enhancement. Resonant wavelength of NPs is characteristic of their size. Since, the NPs are excited by two different wavelengths: one corresponding to excitation wavelength, from the top at λ (=785 nm) and the other corresponding to the reflected wave, from the bottom at λ´ (= λ/n= 785/1.5 = 523 nm), thus different sizes of NPs are excited corresponding to different λ, thereby, increasing the overall light-matter interaction. Identification of an unknown analyte using SERS is determined on the basis of its Raman signature. The Raman peak which lies in the close vicinity of the resonant wavelength of the substrate is more enhanced in comparision to the other peaks.

Commercially available software, Lumerical FDTD solution which is based on Maxwell's partial differential equations has been used to analyse the electromagnetic fields enhancement in Ag/Au mirror based SERS substrate (Figure 1). Simulation results (Fig. 1) illustrate that enhancement increases when we use Au/Ag mirror. Theoretical enhancement factor (EF) is found to be ≈ 8.65×10^5 with Au/Ag mirror, which is 4 times more without mirror.

SERS spectra (Fig. 3) reveal that the presence of Au/Ag coating improves the overall enhancement and can be considered as an example of "energy harvesting", where optical energy which otherwise would have escaped, after getting reflected is reinvested for improving enhancement further.

Keywords: Surface-enhanced Raman scattering (SERS), Au nanoparticles, SERS substrate, Spectroscopy, Chemical sensing.

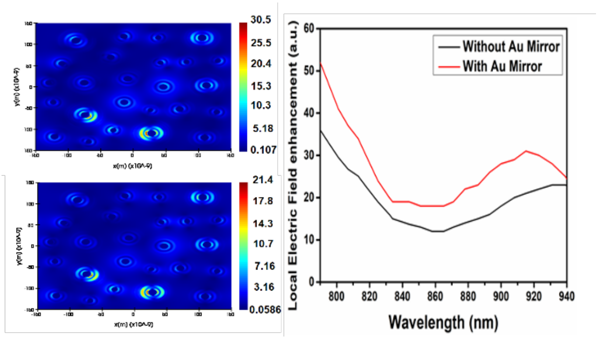

Figure. 1: FDTD results showing electric field profile comparison of with and without Au mirror.

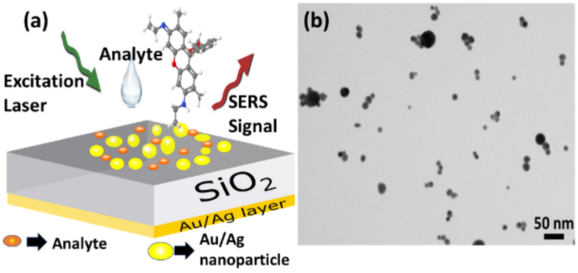

Figure 2: (a) Schematic of SERS substrate (b)TEM image of Au nanoparticles

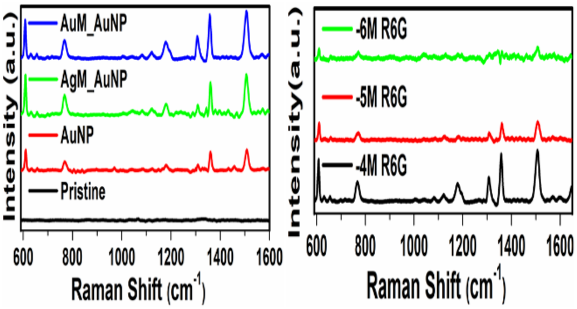

Figure 3: SERS spectra of (a) 10^{-4} M R6G over different combinations of Au/Ag mirror and Au NPs (b) 10^{-4} M, 10^{-5} M, 10^{-6} M R6G over Au NP coated Au mirror.

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NanoMatEn Session III.B: Nanotechnology for Energy/ Nanocatalysis (Part II)

Rational synthesis and catalytic activity of bimetallic Ag/Pt nanoparticles

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Abstract

Metallic nanocatalysts (NCs) have attracted the greatest interest in nanoscience and nanotechnology because of their electronic, chemical and even optical properties (in this case enhanced plasmonic effects) [1]. However, one of the challenges facing NCs is to design new nanomaterials with excellent catalytic performance and low price. Therefore, one strategy is to develop bimetallic NCs composed of two metal elements, that can exhibit synergistic effects between their physicochemical properties and enhanced catalytic activity.

In this context, we designed bimetallic NCs combining the plasmonic metal Ag and catalytic metal Pt. This combination – when efficiently tuned – can lead to plasmonic-driven enhancement of NCs catalytic activities. In addition, these bimetallic NCs often exhibit superior catalytic activity due to the modification of the Pt-Pt atomic bonding distance (i.e., the strain effect). In our work, Ag@Pt NCs were synthesized through seeds-mediated growth with controlled Ag core size and Pt shell thickness [2]. First of all, the Ag seeds (8-14nm) with low size distribution (<10%) are synthesized by chemical reduction by tuning the reaction time and temperature during synthesis (Figure1a-c). The second stage is to tune the Pt thickness (from 1 to 6 atomic layers) by adjusting the ratio between platinum precursor to silver seed concentrations. The Pt shell is mainly heterogeneous (Figure1d-e). The catalytic activity of core-shell Ag@Pt NCs with different Pt thicknesses was tested through a model reaction of reduction of 4-nitrophenol to 4-aminophenol, and compared with that of pure Ag and Pt NPs. Ag@Pt NCs exhibit remarkable enhancement of catalytic activity and stability compared to pure silver or platinum NP (Figure 1f). Furthermore, because of their narrow size and shape polydispersity, Ag@Pt NCs self-organized into 2D and 3D ordered superlattices after drop deposition on a solid substrate. They open a wide range of possible applications especially in the case of catalysis and plasmonic catalysis.

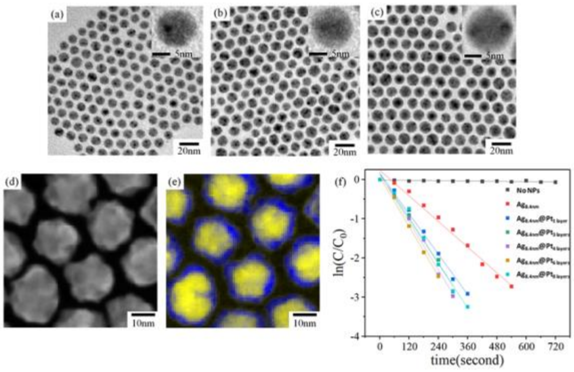

Figure 1: (a-c) TEM images of different Ag seed sizes from 8.4nm, to 10.5nm and 13.3nm, respectively, in inserts higher magnifications (d) STEM- HAADF image of Ag@Pt NPs (e) correspond EELS mapping (in blue Pt and in yellow Ag) (f) Catalytic activity: ln(C/C_0)=f(t) for Ag$_{(8nm)}$ and Ag$_{(8nm)}$@Pt NPs.

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First evidence of lignin-pheomelanin nanostructured UVA driven synthesis of Pummerer's ketones by peroxidase mediated oxidative coupling of substituted phenols

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Abstract:
Pheomelanin (PM), the yellow-to-reddish brown subtype of insoluble melanin pigment is commonly considered as a photosensitizing agent involved in damage of important cellular targets, including DNA nucleobases [1]. Photoexcitation of PM produces high energy singlet state that decays via internal conversion and comproportionation equilibrium with formation of singlet oxygen and superoxide anion. An important issue in challenging the application of PM in organic synthesis is the control of the fate of these reactive intermediates [2]. Recent study from our laboratory has shown that singlet oxygen generated by meso-tetraphenyl porphyrin and blue-LED selectively produced the hydroperoxide derivative of 2-methyltetrahydrofuran (2-MeTHF) in a bi-phasic system. The diffusion of the hydroperoxide to the buffer containing horseradish peroxidase (HRP) fueled the oxidative coupling of phenol derivatives [3]. This procedure avoided the inactivation of HRP by excess of hydrogen peroxide. In this context, singlet oxygen and superoxide anion produced by PM can drive HRP catalyzed oxidative coupling. We also demonstrated that the effectiveness of the process can be in principle favored by lignin nanoparticles (LNPs) playing the dual role of stabilizing support for PM and HRP, as well as redox active platform with boosting activity for the enzyme [4]. Here we report the first evidence that Pummerer's ketones, which are key intermediates for the synthesis of natural drugs, can be synthesized from substituted phenols by a photobiocatalytic PM UVA-driven activation of HRP. The efficacy of the transformation was improved when PM and HRP were embedded into LNPs to afford novel nanophotobiocatalytic platforms. The preparation of these bio-nanodevices included nanoprecipitation and grafting procedures. The novel catalysts were fully characterized, and their structure-reactivity relationships deeply investigated. These results open a new entry for the application of PM based nano-photobiocatalytic systems in organic synthesis.

Keywords: pheomelanin, UV-A radiation, lignin nanoparticles, pummerer's ketone, horseradish peroxidase.

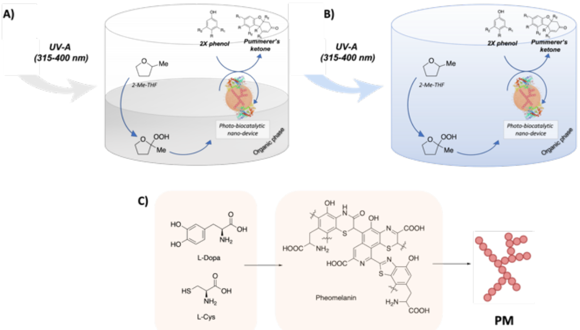

Figure 1: Schematic representation of the synthesis of Pummerer's ketones catalyzed by nanophotobiocatalytic systems in two-liquid-phase systems (2LPs) (Panel A) and mono-phasic systems (MPs) (Panel B). Panel C: Schematic representation of pheomelanin synthesis and structure.

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Facing structural modifications in WO_3 nanomaterials for improved light-responsive textiles

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Abstract:

The search for high-performance photoresponsive textiles has been increasing for several applications, such as anti-counterfeiting, camouflage, UV-protection, and fashion [1]. Photochromic inorganic materials, *e.g.* tungsten(VI) oxide, have the required characteristics for textile applications, including good response to a light stimulus (sunlight/UV radiation), high color reversibility, cyclability and endurance to high temperatures [2]. In this work, several WO_3-based photochromic materials were produced through a low-cost, single-step route, using different types of structure-directing agents. The chemical properties of the structure-directing agent, such as the presence of hydrophilic/hydrophobic groups, positive charge (*e.g.*, cationic surfactant CTAB) or chelating properties (*e.g.*, PVP) led to WO_3 (nano)materials with different morphologies, phase composition, kinetics of coloration and bleaching and even different colors before and after UV light irradiation, as confirmed by electron microscopy, X-Ray diffraction, Fourier transform infrared spectroscopy, Raman spectroscopy, X-ray photoelectron spectroscopy, diffuse reflectance UV−vis spectroscopy and colorimetry. The overall analysis of the materials revealed that the use of PVP as structure-directing agent led to the WO_3 nanomaterial with the best photochromic properties. Afterwards, the influence of the molecular weight of PVP on the photochromic properties of WO_3 was studied. The nanomaterial based on PVP with the lowest molecular weight (WO_3_PVP_L) exhibited the best photochromic performance. Finally, the PVP-based nanomaterials were incorporated on cotton substrates by screen-printing to create photoresponsive fabrics. The light-responsive textile based on WO_3_PVP_L took only 5 minutes to change the color from white to blue upon UV light irradiation, and 5 hours to return to the initial color, presenting a $\Delta E = 28.36$ after irradiation (Figure 1). Furthermore, the use of PVP with higher molecular weight helped to achieve a textile (WO_3_PVP_H@cot) with dual chromism (photochromism and hydrochromism). WO_3_PVP_H@cot rapidly changed its color when irradiated with UV light (4 minutes) and returned to the initial color when placed in the dark after 3 hours, or when immersed in water after 10 seconds. The progress made in WO_3-based photochromic materials is a step forward to the manufacturing of photoresponsive fabrics in the Textile Industry.

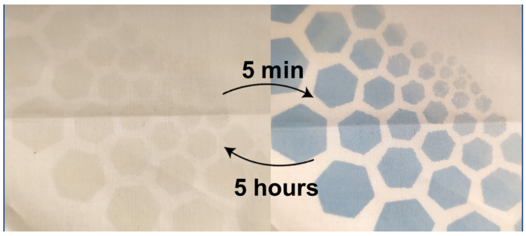

Figure 1: Photographs of the light-responsive cotton fabric WO_3_PVP_H@cot before and after irradiation with UV light ($\lambda = 360$ nm)

Keywords: Tungsten oxide, structure-directing agent, photochromism, light-responsive textiles, screen-printing

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Indium Phosphide Quantum Dots loaded on Mesoporous silica for Visible-Light Photo-Redox Catalysis

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Abstract:

Quantum dots (QDs) or semiconductor nanocrystals with tunable photo-optical and chemical properties are ideal to efficiently photocatalyze many types of relevant reactions for energy conversion and organic synthesis [1,2].
Cadmium sulfide quantum dots are the most studied and have received extensive attention for various photoredox reactions due to their suitable band gap and their high quantum yield. However, their toxicity and the ban of the use of cadmium in the EU have motivated the development of environmentally friendly alternatives.
Indium phosphide is particularly promising thanks to its low intrinsic toxicity and theoretically emitting capacity in the entire range from the visible to the near infrared [3]. However, few reports describe their catalytic activity and feature their poor reusability in homogenous catalysis [4].
The main objective of this study is to demonstrate the potentiality of indium phosphide semiconductor nanocrystals as a heterogeneous photocatalyst by incorporating them in mesoporous silica and graphene materials with high surface area.
The size effect of the InP QDs on the catalytic performances will be studied. Then, we will present here the successful incorporation of the InP QDs in different functionnalized support materials and a first serie of reactions demonstrating their photocatalytic activity.

Keywords: indium phosphide, quantum dots, porous materials, mesoporous silica, heterogeneous photocatalysis, visible-light.

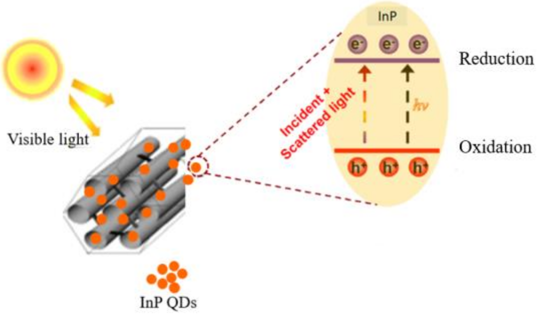

Figure 1: Schematic illustration of QDs-photocatalyzed redox reactions.

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Design and Characterization of Cu and core-shell Cu@ZnO nanocatalysts

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Abstract:

In the recent years, copper and copper-based nanoparticles (NPs) have gained a lot of interest, more particularly in the applied field of catalysis. Indeed, the higher abundance and inexpensiveness of Cu compared to other catalytic metals such as silver, gold, platinum, or palladium for example, make its application as a nanocatalyst highly interesting for industrial applications. A perfect example of copper-based nanocatalyst implemented in industrial processes is the Cu/ZnO/Al_2O_3 system used since the start of the twentieth century for the catalytic conversion of carbon dioxide to methanol.[1]

Many studies have been performed to better understand this catalyst's activity both from theoretical [2] and experimental [3] views on simplified model catalysts Cu/ZnO. However, these studies have failed to consider the effect of particle shape, size, and crystallinity on the catalyst's activity. This is mainly due to lesser number of available studies on Cu NPs synthesis compared to other noble metals (Au, Ag NPs) due to Cu NPs intrinsic susceptibility to oxidation; as well as the Cu (I) and Cu (II) precursors' higher oxidation potentials which necessitates the use of stronger reducing agents and/or the need to perform synthesis at higher temperatures and consequently renders the shape and crystallinity control more challenging.[4] However, few works reported the synthesis of Cu NPs with shape control through the dismutation of copper (I) halides.[5] In this work we report the synthesis of Cu NPs with different shapes and morphologies as well as Cu-core ZnO-shell (Cu@ZnO) NPs through a seed mediated growth method allowing the growth of zinc oxide satellites over the well-defined Cu NPs seeds. The influence of different experimental parameters on copper seed shape and on their crystallinity control was thus studied.

Keywords: nanoparticles, chemical synthesis, copper, zinc oxide, metal-oxide catalyst, seed mediated growth, catalysis, plasmon, carbon dioxide, methanol.

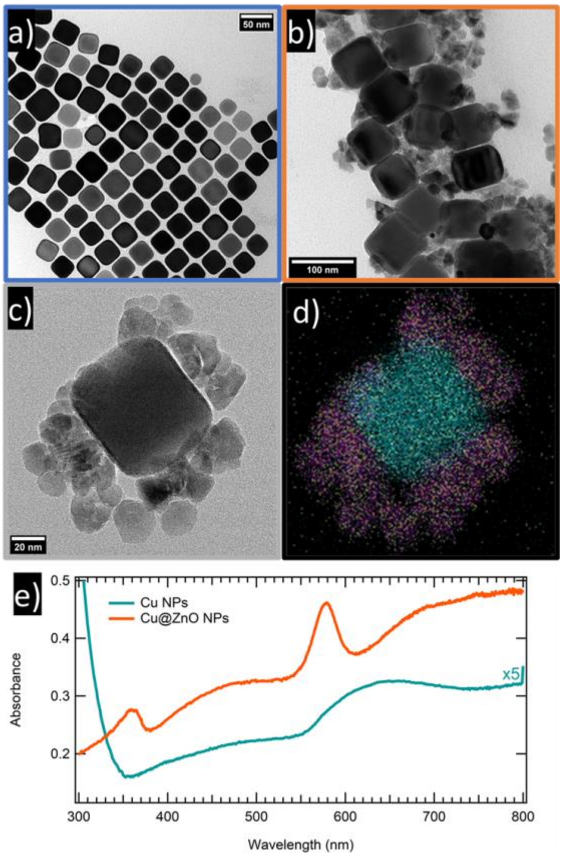

Figure 1: TEM images of cubic a) copper nanoparticles; b) Cu-core ZnO-shell nanoparticles; c) high magnification of a single Cu@ZnO nanoparticle and d) STEM elemental mapping of c) with copper, zinc and oxygen coded as blue, pink and yellow color; e) Corresponding UV-visible absorption spectra of Cu and Cu@ZnO NPs showing intense absorption of Cu seed NPs within the visible range due to the plasmonic properties of copper at the nanoscale.

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NanoMatEn Session III.C: Nanotechnology for Environmental Application / Water treatment

Engineering of nanomaterials and membranes interfaces by Atomic Layer deposition: design, properties and applications

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Abstract:

Nanostructure science and technology are a broad and interdisciplinary area of research and development that has been exponentially growing in the past few years. Engineered nanomaterials are resources designed at the molecular (nanometer) scale to take advantage of their small size and novel properties which are generally not seen in their conventional bulk counterparts. The two main reasons why nanomaterials can have different properties are: (i) the increase of relative surface area and (ii) the quantum confinement effects leading to novel optical, electrical and magnetic behaviors. In order to apply these nanomaterials in different fields and to increase the throughput of nanostructured materials and membranes for energy, environmental and health applications, an efficient control of the interfaces is needed.

Here, we used different synthesis techniques such as atomic layer deposition (ALD) [1], as the main tools for the creation of controlled nanostructured materials and membranes in which the geometry can be tuned accurately and the dependence of the physical-chemical properties on the geometric parameters can be studied systematically in order to investigate their performances in energy, environmental and health applications. We will show examples of how these methods can be used to create single nanopores for sensing, membrane for gas purification [2,3], osmotic energy harvesting [4] and water treatment as well as sensors and biosensors [5], in which the performance varies with the nanostructures/interfaces..

Keywords: Atomic Layer Deposition, membrane, gas sensing, gas separation, biosensing, water treatment.

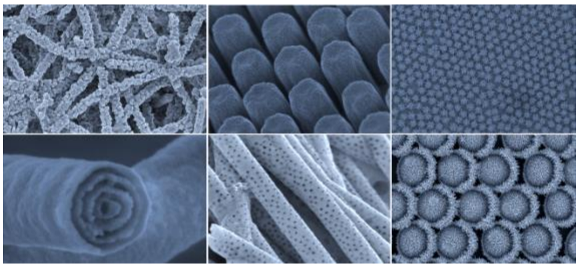

Figure 1: Design of nanomaterials for energy, environmental and health applications.

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Fabrication of electrospun nanofibers based membranes and their use for CO_2 capture

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Abstract:
One of the huge threats our planet is facing is the climate change. Catastrophic effects predicted to result from climate change such as global warming, melting of glaciers, increase of the sea level, species disappearance, pollution, economic disruption, and starvation needs to be mitigated. In order to overcome these problems, the effects of greenhouse gasses, especially CO_2 have to be mitigated. One promising technology is CO_2 capture, transportation and storage (CCTS). CO_2 capture technologies are available on the market, but they have generally high costs, accounting for more than 70% of the total costs of a full CCTS system. Novel materials and technologies need to be developed for CO_2 capture and storage in order to make this technology more cost efficient. Thanks to their properties (e.g. lower capital and processing costs, smaller unit size, simple operation, better energy efficiency, easy up-scalable, lower environmental impact, process flexibility, continuous operation) membranes proved to be a viable technical approach for CO_2 capture. The innovative solution proposed is to use the electrospinning technique to produce nanofiber-based membrane. The main property of the electrospun nanofiber that is be exploited is their very high surface area. Optmisation of the electrospinning process parameters was done for polimeric nanofibers without and with additives. Further post-processing (e.g. calcination) of the nanofibers will highly increase the porosity, thermal stability and chemical characteristics. Among the main benefits of nanofiber-based membranes their high absorption capacity for CO_2 stable performance during absorption/desorption cycling has to be highlighted.

Keywords: electrospinning, nanofibers membrane, CO_2 capture.

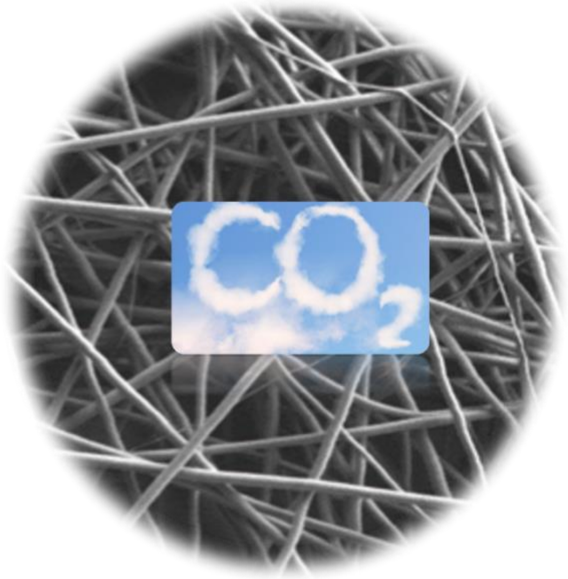

Figure 1: SEM image of electrospun nanofibers based membrane used for CO_2 capture.

Design of nanocomposite based on halloysite for water treatment

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Abstract:
Due to their unique physical properties, chemical stability, high activity, strong oxidation capability, and numerous potential applications in solar energy, Titanium oxide (TiO_2) nanofibers are receiving considerable attention in environmental applications. Here, we designed and synthesized halloysite-TiO_2 nanocomposites fibers by combining electrospinning and sol-gel method. The halloysite (HNTs) used was extracted from Tamra (NW Tunisia). The halloysite and TiO_2 ratios have been optimized and the obtained materials were characterized using thermogravimetric analysis (TGA), X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Energy-dispersive X-ray spectroscopy analysis (EDX), Raman spectroscopy, N_2 surface area analysis by BET and X-ray photoelectron spectroscopy (XPS). The results confirmed the incorporation of HNTs into Titanium oxide nanofibers and indicated the removal of methylene blue and acetaminophen at neutral pH using the composites nanofibers as photocatalyts under UV and Visible irradiation >91% (Figure 1). In addition, reusability tests showed a good stability over 5 cycles under visible light. Moreover, toxicity and scavenging tests were carried out to identify reactive radicals responsible for the degradation. Overall, the TiO_2 /HNTs nanofiber is an effective nanocomposite for the removal of organic dyes and pharmaceutical compounds from wastewater.

Keywords: halloysite nanotubes, TiO_2 nanofibers, electrospinning, photocatalysis, methylene blue, acetaminophen.

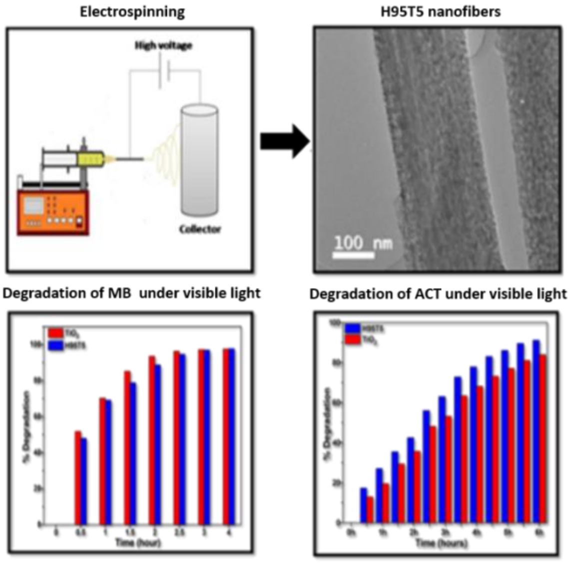

Figure 1: Figure illustrating the synthesis of one-dimensional nanocomposite (halloysite-TiO_2) with photocatalytic degradation of ACT and MB under visible irradiation.

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Development and characterization of porous calcium copper titanate membranes for water treatment

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[2] Laboratoire de Chimie-Physique Macromoléculaire (LCPM), Lebanese University, Jdeidet, Lebanon

Abstract:

Human health and the ecology of the environment are affected by water pollution worldwide. The ecological and sustainable solution to global pollution is important. Using solar light in conjunction with a catalyst is an attractive approach for degrading pollutants, based on the generation of hydroxyl radicals (• OH), which are nonselective and highly oxidizing species capable of mineralizing organic compounds (figure 1). The most important parameter in the photoelectrocatalysis process is the performance of the semi-conductor used as photo-anode.

In this study, we are interested in the perovskite oxides due to their unique structure properties, high chemical stability and excellent optical characteristics. A porous membrane of calcium copper titanate ($CaCu_3Ti_4O_{12}$ (CCTO)) with different percentage of polymethyl methacrylate (PMMA) used as pore-forming agent has been synthesized.

Different characterization methods were used to investigate the properties of the synthesized membrane: (i) Scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD) for textural and structural properties; (ii) UV-Vis diffuse reflectance and photoluminescence spectroscopies for optical properties; (iii) Cyclic voltammetry measurement, and impedance spectroscopy for electrochemical activity.

CCTO nanocomposites were used as anode in an electrochemical cell to treat a synthetic effluent containing paracetamol which was tracked using high performance liquid chromatography (HPLC) and TOC analysis to characterize degradation and mineralization efficiency respectively. Peroxymonosulfate (PMS) were added to enhance the degradation efficiency of paracetamol. Finaly the acute toxicity (Microtox) of potential by-products following the degradation was also investigated.

Keywords: Waste water treatment, photoelectrocatalysis, perovskite oxides, calcium copper titanate, paracetamol degradation.

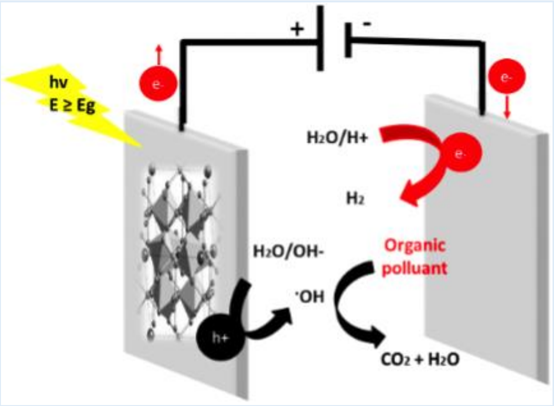

Figure 1: Photoelectrocatalysis process for degradation of organic pollutant using CCTO as photoanode.

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Reiterative usage of bi-layered nanocrystaline carbon-doped TiO_2 and Ni particles for the photocatalytic water treatment

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Abstract:
Photocatalytic water treatment is considered as one of the most promising environmental friendly technologies which could be used for the decontamination of both organic and inorganic pollutants [1]. Up to now, in laboratory tests arguably the best photocatalytic treatment results (both under UV and visible light irradiation) were obtained using various modifications of nanocrystalline TiO_2 powder photocatalyst [2]. However, in order to make it more suitable for the practical applications, it is highly desirable to make the photocatalyst convienient for the reiterative usage. The most widely applied solution is to imobilise the nanocrytalline photocatalyst powder/particles on larger elements which could be easily manipulated by the conventional methods [3]. However, this approach has some limitations. For example, with large support elements it can be hard to distribute the immobilized photocatalyst evenly throughout the treated media. Accordingly, in current study we tested the opposite approach and tried to produce microscopic photocatalyst particles with significant feromagnetic properties which would allow their collection and manipulation by the magnetic field. Such ferromagnetic photocatalyst particles were produced in two steps. First, we used successive magnetron sputter deposition of nanocrystalline Ni and carbon-doped TiO_2 films on soluble salt grains (Figure 1a). Then, we dissolved the supportive salt grains in water and observed the bi-layered photocatalyst particles consisting of Ni layer on one side, and carbon-doped TiO_2 layer on the other side. The structure of bi-layered photocatalyst particles was characterized by XRD, SEM and XPS techniques. Whereas, their photocatalytic activity and its long term stability was evaluated by using aquaeous dye solution bleaching method. The bilayered photocatalyst particles were relatively light and during the bleaching test inside the glass vessel were easily mixed by the conventional magnetic stirrer (Figure 1b). Then the magnetic stirrer was switched off, the photocatalyst particles reacted to the magnetic field of the magnetic stir bar and adherred to its surface (Figure 1c). This was very convenient for the photocatalyst removal from the solution (together with the bar) and for the reiterative usage of the same photocatalyst material for the treatment of new portions of contaminated solutions.

Keywords: TiO_2, photocatalysis, photocatalyst, nanomaterials, reactive magnetron sputtering, photocatalytic bleaching, ferromagnetic coatings, nanostructured coatings, water technologies, environment.

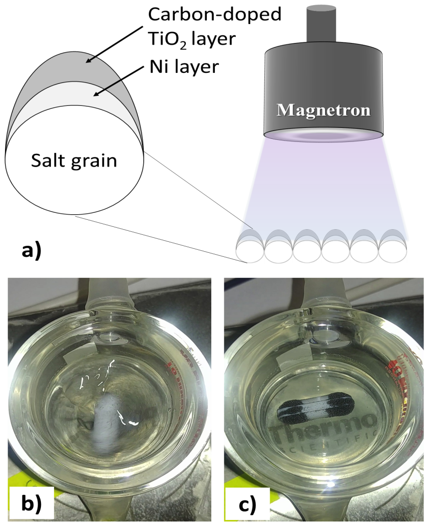

Figure 1: Experimental scheme of the nanocrystaline bi-layered carbon-doped TiO_2 and Ni photocatalyst particles formation (a), the view of the stirred photocatalyst particles during the performance of photocatalytic bleaching test (b), and collection of used photocatalyst by the magnetic field of the strir bar after bleaching test (c).

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Conjugated microporous polymers using a copper-catalyzed [4 + 2] cyclobenzannulation reaction: promising materials for iodine and dye adsorption

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Abstract:

A design strategy is disclosed to synthesize conjugated microporous polymers (CMPs) using a versatile copper-catalyzed [4 + 2] cyclobenzannulation reaction, which employs a diphenylethynyl terephthalaldehyde derivative 3 with a series of triptycene-based diethynyl aryl building blocks 2a–e. Investigation of the intrinsic microporosity properties of CBP1–5 using nitrogen adsorption measurements reveals Brunauer–Emmett–Teller (BET) surface areas up to 794 m2 g−1 and average pore volumes reaching 0.63 cm3 g−1. Inspection of the adsorption properties of the graphitic-like polymers CBP1–5 divulges their high iodine uptake with a maximum of 166 wt%. Moreover, the target polymers CBP1–5 prove their efficiency as selective dye adsorbents by removing up to 100% methylene blue over methyl orange from aqueous solution.

A comparison of unmodified and sawdust derived-cellulose nanocrystals (CNC) modified polyamide membrane using zeta potential and permeability

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Abstract:

The aim of this work was to investigate the efficiency of the surface modification of a polyamide membrane using zeta potential and water permeability. The polyamide membrane was modified with sawdust derived-cellulose nanocrystals (CNC) and compared with an unmodified membrane. The two membranes were prepared using the interfacial polymerization technique. The aqueous phase was 1 wt% m-phenylene-diamine (MPDA) in deionized water. The organic phase was 0.5wt% of trimesoyl chloride (TMC) in hexane. For the modified membrane, 0.21% wt CNC was introduced into the aqueous phase. For both membranes, 0.4 wt % sodium hydroxide was added to the aqueous phase to act as an acid acceptor. Each membrane was cast on a supporting UF membrane having a molecular weight cut off (MWCO) of 100 kDa. Both modified and unmodified membranes were investigated for zeta potential and water permeability. The zeta potential measurement was carried out using SurPASS 3 instrument. The water permeability test was carried out with deionized water at 7 bar using a dead-end test cell. For both membranes, the negative zeta potential decreased at a high pH and the isoelectric point shifted towards the acidic range. This is an indication of the hydrophilicity of both membranes. However, the zeta potential of the modified membrane was more negative than that of the unmodified. This is an indication of the successful modification of the membrane. This was also reflected in the water permeability of the modified membrane that was higher than the unmodified membrane.

Keywords: Cellulose nanocrystals, polyamide, membrane, interfacial polymerization, zeta potential, water permeability.

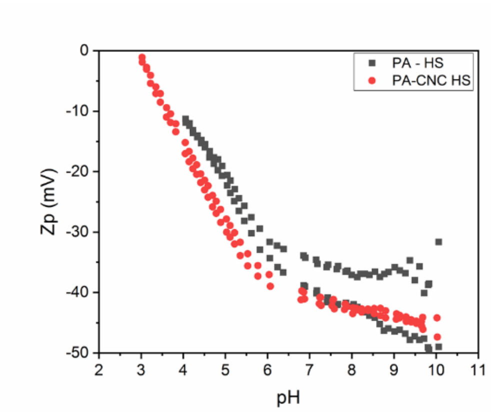

Figure 1: pH dependence of zeta potential for unmodified membrane (PA) and the mebrane modified with sawdust-derived cellulose nanocrystals (PA-CNC). The figure shows a change in the surface charge as a result of the modification

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Nanotech / Biotech Session III.C: Nanotechnology for Drug and Gene Delivery

2D hybrid MnAl-fluorouracil nanotheranostic construct with controlled morpho-structural properties

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Abstract:
In this contribution, the development of a nanotheranostic agent based on manganese and fluorouracil (FU) anticancer drug agent, which exhibited increased longitudinal relaxivity (r1) and strongly pH-controlled delivery of FU is duscussed. The manganese, which fully replaced magnesium, was rationally included in a two-dimensional layered double hydroxide (LDH; Mn/Al = 2/1) by co-precipitation (CP) at low saturation. The anticancer drug was strategically introduced in the layered solid by two synthetic approaches, i.e., CP at low suprasaturation and CP coupled with ion-exchange (IE).

The materials were characterized by AAS, XRD, N_2 physisorption, FT-IR, SEM, TEM and TG in order to assess their chemical composition, structure, texture and morphology. The oxidation state of manganese was characterized by DR UV-vis and XPS. The results of physico-chemical characterization revealed high-quality 2D materials in which manganese mainly exists as Mn^{2+} and Mn^{3+} while the mass loading of FU was of 6.96 and 5.28% for the samples prepared by CP and CP coupled with IE, respectively. The ability to retain proteins, as a key obstacle in the intravenous delivery of nanomedicines, was studied by UV-Vis spectroscopy and polyacrylamide gel electrophoresis (SDS-PAGE) using a fixed bovine serum albumin (BSA) solution of 0.4 mg/mL at pH 7.4 and different LDH concentrations (0.5, 1, 1.5, and 2 mg/mL). UV-Vis and SDS-PAGE results showed similar results with up to 17.42% and 21.55 %, respectively, BSA adsorption after 2 h incubation at room temperature for LDH 1 mg/mL. Yet, washing had removed the most part of the adsorbed BSA, clearly indicating the slight protein bonding on the LDH surface. The relaxivities r_1 and r_2, obtained on a 1.0 T apparatus pH 7.4 and 6.4 showed a noteworthy improvement, particularly for r_1 at pH = 7.4, for which a value of 1.772 mM^{-1} s^{-1} was obtained. The release of FU from MnAl LDH was severely controlled by pH while the mathematical models used to fit the data revealed a quasi-Fickian diffusion of the FU discharge. Interestingly, the formation of FU-Mn complex at acidic pH (6.4) was noticed based on the FT-IR performed on the solid recovered after the controlled release experiments. The formation of such a complex is improtant because it might influence the clinical effects of the developed nanomedicines based on transition metals.

Keywords: layered double hydroxides, managanese, fluorouracil, nanotheranostic, MRI, protein corona.

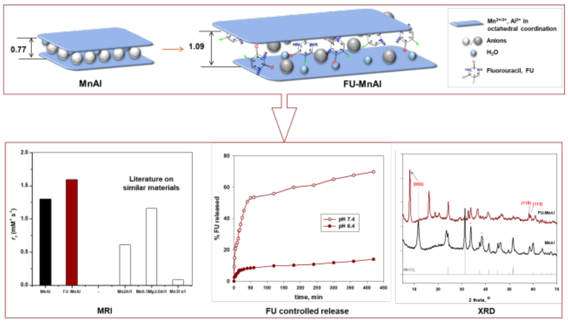

Figure 1: *Up*: The accomodation of FU into the interlayer space of MnAl LDH aiming to develop a theranostic nanoconstruct. *Down*: XRD shows the formation of the LDH structure hosting FU, which release is strongly affected by the pH. Incorporation of Mn into the octahedral sheets of LDH significantly increased the value of longitudinal relaxivity, r1, as compared with those obtained for similar materials at higher power.

Acknowledgments: This work was supported by a H2020 grant – ERA-Chair, no 952390 and a grant of the Ministry of Education and Research, CNCS/CCCDI - UEFISCDI, project number PN-III-P3-3.6-H2020-2020-0105/35/2021.

Magnetic iron oxide nanoparticles for the delivery of thermal therapy for the treatment of Adrenocortical Carcinoma

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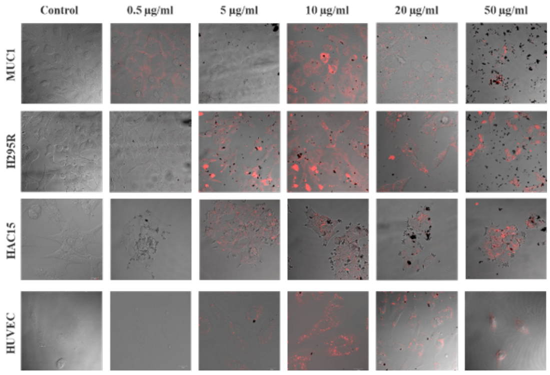
Abstract:
To minimise damage to surrounding tissues, targeted delivery of therapeutics to the tumour is highly desirable, and the development of nanotechnology has shown promising results. Magnetic iron oxide nanoparticles (MIONPs) have been gaining traction over the years for applications such as drug delivery, molecular imaging and delivering hyperthermia for treatment of various cancers (1). MIONPs have great therapeutic potential as they can be produced in various sizes and shapes, with the ability to modify the surface by coating the nanoparticles. MIONPs have the ability to be activated by external magnetic field to generate heat and to cause hyperthermia (2).

Translationally, the delivery of thermal therapy offers an option for minimally invasive definitive treatment of primary aldosteronism, an endocrinopathy of aldosterone excess/dysregulation which represents the commonest secondary form of hypertension. In this study, MIONPs have been used at different concentrations to evaluate nanoparticle uptake and rate of uptake by adrenal cortical and endothelial cells, as well as gain understanding of the location of nanoparticles within the cell.

Magnetic iron oxide nanoparticles (MIONPs) were provided by Kansas University. Adrenal Cortical cell-lines (MUC1, H295R and HAC15) and Endothelial cell-line (HUVEC) were used in this study. MIONPs were added at concentrations of 0.5, 5, 10, 20 and 50 µg/ml to the cells and incubated overnight. MIONP uptake efficiency, rate of uptake and cytotoxicity was assessed by Flow Cytometry. Confocal Microscopy was used to image the cells following MIONP incubation. Cellular proliferation was assessed by Xcelligence system and alamarBlue. Cellular respiration was assessed by "Seahorse" technology. MIONP location within the cells was assessed by transmission electron microscopy (TEM).

Follwoing overnight incubation with MIONPs, Flow Cytometry showed significant uptake by MUC1, HAC15 and HUVEC cells at 10 µg/ml MIONP concentration. Confocal and TEM images revealed MIONPs in the cytoplasm and in the vesicles for all cell types (**Fig. 1 and 2).** Live Confocal imaging showed MIONP phagocytosis specific uptake by the HAC15 cells.

Keywords: Nanoparticles, MIONP, MUC1, HAC15, H295R, HUVEC.



Figur 1: Confocal images of MUC1, H295R, HAC15 and HUVEC cells incubated with MIONPs at different concentrations overnight. The uptake of MIONP plateaud at a concentration of 10 µg/ml. MIONPs (in red) shown inside the cytoplasm.

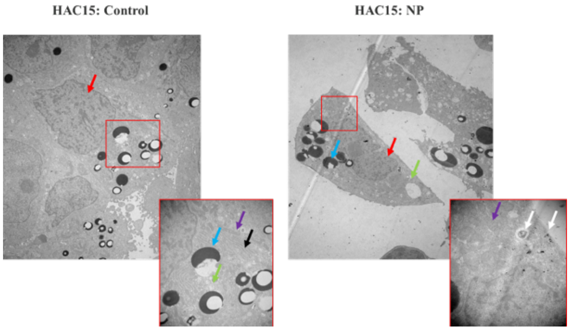


Figure 2: TEM images of HAC15 cells incubated overnight with the optimal MIONP concentration of 10 µg/ml. TEM revealed MIONPs in the cytoplasm and vesicle of the cell. White arrow indicating the MIONPs, blue arrow indicating the lipd droplets and red arrow indicating the nuclei.

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pH-Responsive PAMAM Dendrimers Encapsulating *Peganum harmala* Alkaloids and Tannic Acid with Improved Anticancer Activities as Compared to Doxorubicin

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Abstract:
This work aims to develop a pH-responsive dual-loaded nanoplatform based on generation 3 PAMAM dendrimer (G3) loaded with Tannic acid (T) and Peganum harmala alkaloids (H) for the treatment of breast cancer. In this regard, G3 nanoparticles (NPs) loaded with either DOX, T, H, or dual-loaded with T-H were prepared. The average particle sizes of the designed DOX@G3, H@G3, T@G3, and T-H@G3 NPs were 78±5.1, 122±3.7, 141±2.8, and 192±1.9 nm, respectively. All the prepared NPs exhibited high positive surface charges and high entrapment efficiencies. Release studies showed the ability of the NPs to release their cargo selectively in the cancerous cell microenvironment (pH of 5.5) via a pH-triggered mechanism while maintaining stability at physiological pH of 7.4. Furthermore, the T@G3, H@G3, and T-H@G3 NPs exhibited remarkable cytotoxic activities against breast adenocarcinoma (MCF-7) cells with IC_{50} values of 4.5, 2.6, and 1.7 µg/mL, respectively; as compared to DOX@G3, free DOX, free H and free T (IC_{50} values of 4.7, 6.75, 5.8 and 7.2 µg/mL), as presented in Figure 1. In conclusion, dendrimers loaded with *Peganum harmala* alkaloids and tannic acid hold the potential for effective treatment of breast cancer.

Keywords: Dendrimers, polyamidoamine (PAMAM), Doxorubicin, *Peganum harmala* alkaloids, Tannic acid, breast cancer.

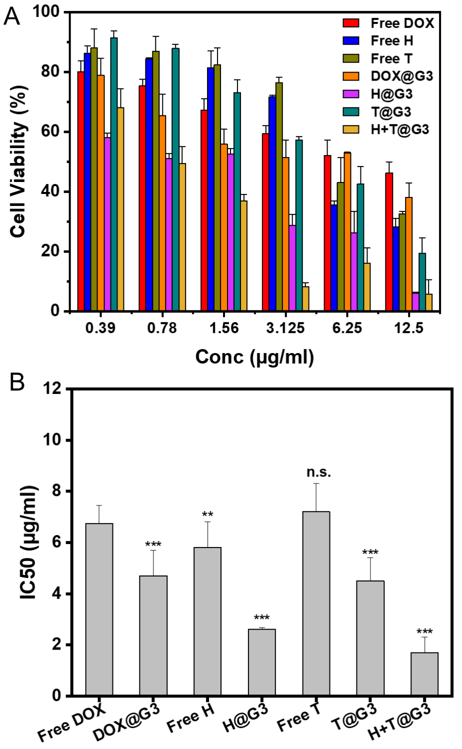

Figure 1. (A) The cytotoxicity and (B) IC50 values of free DOX, H, T, DOX@G#, H@G3, T@G3, and T-H@G3 at various concentrations using MTT assay in MCF-7 cells when incubated for 24 h.

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Multifunctional Polymer-Nanoparticle Composite for Wound Care Applications

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Abstract:

Wound healing is a complex physiological process that is broadly classified in four overlapping cellular phases - haemostasis, inflammation, proliferation, and remodelling. However, the events such as uncontrolled bleeding, microbial infections, and pain adversely affect the therapeutical control of a patient and the normal healing process. Currently used wound care clinical protocols prescribes the use of pain relief, hemostatic and antimicrobial drugs or devices, and consider usually the use of special wound dressings available in the market. Those are either very expensive and/or do not comprehensively address the normal healing process.

Herein, we present preparation of a multifunctional polymer-nanoparticle composite that is comprised of an antimicrobial core, layer-by-layer (LBL) deposited hemostasis promoting polymers and pain-relieving attached drugs (Fig. 1). The Nanocomposite core at a very low concentration exhibits broad spectrum bactericidal activity against various Gram-positive and Gram-negative bacterial species as well as some yeast and viruses. Antimicrobial core was coated with known hemostasis promoting polyelectrolytes using LBL method and simultaneously loaded with different pain-relieving drugs on to the polymer layers. The pain-relieving drugs presented a two-step kinetic profile of fast release within first few hours followed by a sustained release over several hours. Finally, to demonstrate the potential application, a typical cotton gauze wound dressing, was embedded with multifunctional nanocomposite.

Keywords: wound healing, nanocpmposite, antibacterial, drug release.

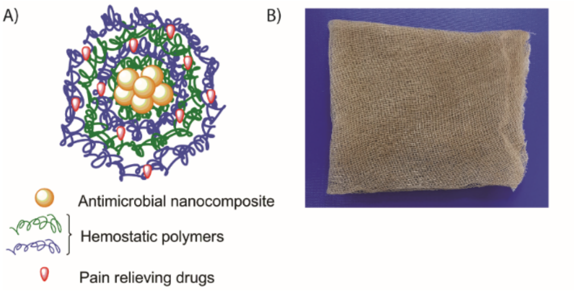

Figure 1: A) Schematic representation of the multifunctional nanocomposite; B) Proof of concept for coating multifunctional nanocomposite on a first aid wound dressing gauze.

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Multifunctional nanogels containing SPIONs and miRNAs for wound healing and skin regeneration applications. The EuroNanoMed project TENTACLES

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Abstract:

Despite recent clinical advances in wound healing, especially on novel materials able to protect the wound and promote healing at the same time, several systemic and local factors can disrupt the physiologic healing process. Therefore, the development of novel therapeutically active wound dressings which provide the wound protection from 'environmental' effects as well as wound healing promotion has an advantageous potential for clinical applications [1]. Nanotechnology as a rapidly expanding multidisciplinary scientific field opens the door to innovative therapeutical approaches in the skin repair process. Nanotechnology-based materials incorporated into scaffolds allow the creation of nanocomposite smart materials with unique physicochemical and biological properties promoting skin regeneration. The aim of the TENTACLES project is to develop an innovative multifunctional nanogel that brilliantly integrates the protective (polymer-based nanohydrogel) and healing functions (iron oxide nanoparticles and targeted miRNA) within one nanocomposite smart structure. The heating-mediated stress stimuli via magnetic iron oxide nanoparticles mild fluid hyperthermia (MFH) promote heat shock protein (HSP) induction involved in fibrogenesis [2], extracellular matrix (ECM) production and transforming growth factor-β1 (TGF-β1) activation [3, 4], which is essential to fibrosis. Additionally, miRNA molecules, the key players in the wound repair and regeneration processes [5], contribute to the promotion of the wound healing process via expression modulation of particular genes. The proposed innovative nanocomposite smart nanohydrogel provides revolutionized wound healing therapeutical strategy particularly for diabetic or long stay recovered patients. No evidence has been reported so far about the use of mild hyperthermia and miRNAs in the promotion of skin repair and regeneration.

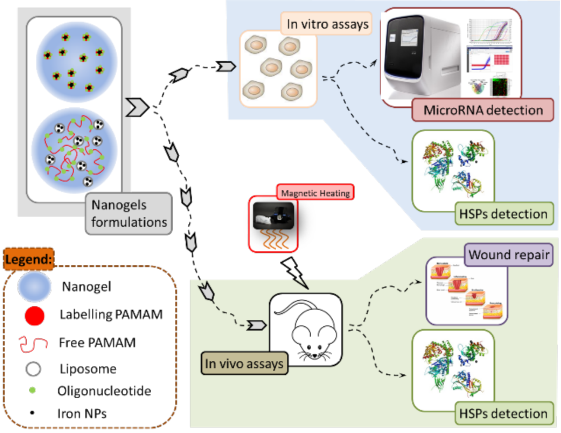

Figure 1: Graphical experimental workflow

To date, many polymeric materials have been clinically used for wound dressing [6], but, actually, none of them contains multiple 'active' therapeutic molecules at the same time. Nanogels are polymeric drug delivery systems made by one or more molecules linked together by physical and chemical linkages to form hydrogels [7]. Nanogels, referred also as hydrogel nanoparticles, have the characteristics of both hydrogels and nanoparticles (NPs) [8]. Nanogel drug delivery systems are able to protect effectively active substances from oxidation and degradation [9], therefore macromolecular drugs and therapeutic agents such as siRNA [10-12], DNA [13] and oligonucleotides [14,15] can be stably loaded into these systems. For this purpose, we preliminary prepared and characterized several commercial (Pluronic-F127 and Ca^{2+}-crosslinked alginate), and synthetic biogels (Gelatin-, chitosan- and chondroitin sulphate-methacrylates) containing iron nanoparticles and miRNAs. We analyzed the differences of these biogels and demonstrated their ability to retain the iron oxide NPs within their bulk structure and release miRNAs at the same time. Preliminary results showed the great ability of alginate to entrap both iron oxide nanoparticles and miRNA, and the efficiency of GelMA and pluronic biogels to differently release miRNAs and NPs. Moreover, these hydrogels are also able to heat by electromagnetic irradiation, owing to the presence of iron oxide NPs. These biogels have therefore multifunctional properties and by modulating each of these properties is it possible to create even more complex systems.

In this contribution, we will illustrate the potential application of these biogels, their physicochemical properties and toxicity profiles on skin models (cells and organoids), and the delivery of selected miRNAs for the modulation of important pathways related to skin regeneration.

Finally, we think that the coupling of different techniques to wound healing, could pave the way to novel industrial opportunities and lead to the realization of patient-oriented devices, aimed at improving the general health status of patients.

Keywords: Nanogel, Wound healing, miRNAs, Heat shock proteins, Iron oxide nanoparticles, Thermal treatment.

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Synthesis and characterization of novel temperature-responsive biogels for microRNA delivery in wound healing applications. The TENTACLES project

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Abstract:
Despite recent clinical advances in wound healing, especially on novel materials able to protect the wound and promote healing at the same time, several systemic and local factors can disrupt the physiologic healing process. Therefore, the development of novel therapeutically active wound dressings which provide the wound protection from 'environmental' effects as well as wound healing promotion has an advantageous potential for clinical applications [1]. Nanotechnology as a rapidly expanding multidisciplinary scientific field opens the door to innovative therapeutical approaches in skin repair process. Nanotechnology-based materials incorporated into scaffolds allow creation of nanocomposite smart materials with unique physicochemical and biological properties promoting skin regeneration. The aim of the TENTACLES project is to develop an innovative multifunctional nanogel that brilliantly integrates the protective (polymer-based nanohydrogel) and healing functions (iron oxide nanoparticles and targeted miRNA) within one nanocomposite smart structure. The heating-mediated stress stimuli via magnetic iron oxide nanoparticles mild fluid hyperthermia (MFH) promote heat shock protein (HSP) induction involved in fibrogenesis [2], extracellular matrix (ECM) production and transforming growth factor-β1 (TGF-β1) activation [3, 4], which is essential to fibrosis. Additionally, miRNA molecules, the key players in the wound repair and regeneration processes [5], contribute to promotion of the wound healing process via expression modulation of particular genes. The proposed innovative nanocomposite smart nanohydrogels provide revolutionized wound healing therapeutical strategy particularly for diabetic or long stay recovered patients. No evidence has been reported so far about the use of mild hyperthermia and miRNAs in promotion of skin repair and regeneration. Moreover, the coupling of different techniques to wound healing, could pave the way to novel industrial opportunities and lead to the realization of patient-oriented devices, aimed at improving the general health status of patients.

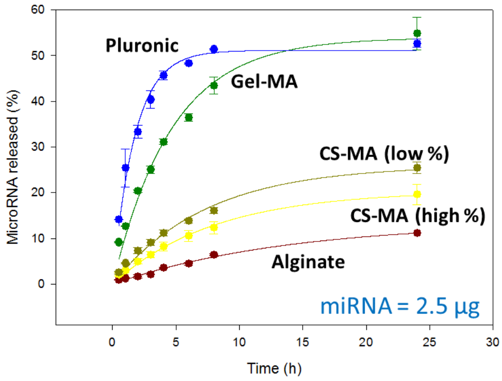

Figure 1: miRNA release from different biogels up to 24h from the initial incubation.

Here, we will show the synthesis and the physico-chemical characterization of a series of new biogels and their miRNAs release properties.

Keywords: Nanogel, Wound healing, miRNAs, Heat shock proteins, Nanoparticles, Thermal treatment

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Nanostructured semiconductor $CuO_{(1-x)}ZnO_x$ nanocomposite with a broad spectrum antibacterial activity and its application in medical devices and acrylic paints

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Abstract:

Hospital-acquired infections or nosocomial infections results in patients suffering, mortality and a substantial burden on the medical system. Recent increase in the nosocomial infections is tightly linked to the observed increase in antimicrobial resistance, which has become a global health threat in the past years.

One promising approach is based on nanotechnology; apparently the specific organization of atoms at the nanometer scale can enhance the antimicrobial activity of known antimicrobial agents or even provide new antimicrobial activity to regular materials.

Probably the most studied antibacterials are Silver nanoparticles (AgNPs). However, lately regulatory agencies have been expressing concerns towards AgNPs due to their cytotoxicity, that is leading to focus the efforts toward more biocompatible antimicrobial materials. Another factor to be considered is the ability to produce those material in large scale enough to support their industrial application in high quality standards and at a low cost .

The present work describes an innovative material comprising of a mixture of metal oxides nanocomposite semiconductor with high nanoporosity and special agglomerate structure that confere remarkable properties as an antibacterial agent. Some of the interesting characteristics of the material are, n-type/p-type hetherojuntions, narrow band gap, slow dissolution and high specific surface area for an improved Reactive Oxygen Species (ROS) release, bacterial-particle interactions and therefore high bacterial toxicity and high biocompatibility. Bactericidal activity is governed by synergetic combination of electrostatic interaction of nanocomposite with bacterial cell envelope and simultaneous generation of ROS. In addition, it can be manufactured at a scale of around 100 Kg/day in a high quality and at a marginal cost.

Both physicochemical properties and its broad spectrum activity against bacteria, viruses, and fungi makes it possible to apply it in various medical devices and industrial areas such as wound dressing, antibacterial barrier, pharmaceutical formulations, non-wouven fabrics, and paints, etc.

Keywords: Antibacterial resistance; medical devices; metal oxide; nanocomposite.

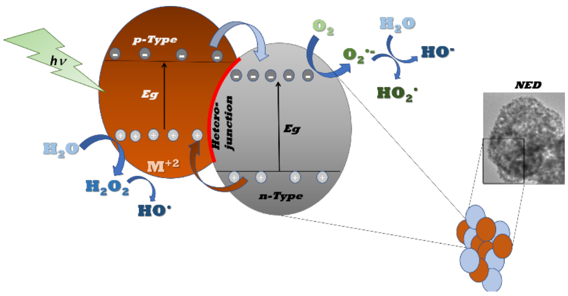

Fig 1: schematic representation of ROS release proposed mechanism in the material.

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Assessment of occupational exposure to nanoparticles during the development of enhanced materials for metal additive manufacturing

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Abstract:
The use of nanomaterials (NMs) in metal additive manufacturing (MAM), or more commonly known as 3D-printing, is enabling the development of new solutions, especially in aerospace, automotive and metal manufacturing industries, by overcoming existing limitations of the traditional processes. The emergent use of the nanotechnology in MAM is driving many benefits, such as the reinforcement of the mechanical properties of the final printed metal parts. Additionally, the inclusion of the nano-scale materials can be a sustainable route for low waste production in MAM industry.

The present work relies in the risk assessment activities planned within the scope of ISQ's collaboration in the MULTI-FUN project. MULTI-FUN is a Horizon 2020 project focused on MAM technology to overcome some of the restrictions present in the current technology. One of the strategies consists in the development of new materials using nanotechnology, allowing the integration of heat sink materials with improved thermal conductivity, a high degree of integral design, e.g. insulated electrical conductors embedded in complex shaped metal structures and adding sensing and data transfer capabilities into metal parts for condition and structural health monitoring. Linking to the 17 global goals of the United Nations for sustainable development [1], the safe and sustainable development of the MULTI-FUN materials involving nanotechnology is critical to ensure compliance with regulation and, consequently, attain an effective deployment.

Despite it is recognized that in the engineered nanomaterials arise many functional advantages from their exclusive physical and chemical properties, there is also a growing concern on the possible health risks resultant from the occupational exposure to these new materials. For instance, several toxicity studies have been reporting the high potential for specific adverse health effects, such as lung inflammation and cardiovascular complications [2-4].

The exposure assessment to nanoparticles (NPs) emissions poses unique challenges in the field of occupational health and safety. The lack of occupational exposure limits (OELs) for engineered nanomaterials, as a consequence of the limited knowledge regarding the real extension of the exposure to NPs in the workers' health, is leading to alternative qualitative assessments to find risk mitigation or control measures. Examples are the Tiered approach (described in EN 17058, 2018) [5] for nano-objects and their aggregates or agglomerates (NOAAs), or risk-banding tools, such as the Stoffenmanager Nano, that helps to prioritize risks and assist the implementation of control measures [6]. Therefore, the monitoring of airborne nanoparticles is of great importance to clarify the level of exposure a worker may be subject while performing a certain activity and whether such exposure poses a risk to their health. The measurement of coarser airborne particles has been typically assessed through mass concentration, which for the case of the nanoparticles is not suitable, due to their high reactivity and wide surface area [7]. Currently, there are no established metrics for the exposure assessment to airborne nanoparticles, but other metrics such as number concentration and, especially, the lung deposited surface area (LDSA) are recognized to be more suitable metrics of dose for predicting pulmonary inflammation [8].

The present work envisioned to assess NPs emissions from experimental procedures carried out indoors of a research institute, aiming the exposure assessment at the MULTI-FUN material stage development. The implemented experimental procedures, *e.g.* ball milling and physical vapor deposition, were selected to obtain metal powders or wires, nanostructured or nanofunctionalized, with enhanced properties to be used in MAM processes. The exposure assessment was carried out using 2 different portable equipment: DiscMini and Nanoscan SMPS. This

methodology allows to assess a broader range of metrics, through different methods of monitoring, enabling a more detailed evaluation of the nanoparticles in the working air environment. Additionally, the present work includes a reflection on the current guidelines of nanoparticle exposure assessment.

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Wound dressing based on cellulose sponges incorporated with curcumin-β-cyclodextrin inclusion complex and chitosan

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Abstract:

The price of wound care products in the international market was estimated at US$19.8 billion in 2019 and is expected to reach US$ 24.8 billion by 2024. Therefore, the treatment of wounds and its efficiency significantly challenge to economic healthcare. In this research, the cellulose sponges with curcumin-β-cyclodextrin inclusion complex (Mx) and chitosan (CS) were fabricated for use as wound dressings. Morphological appearances, mechanical properties, water retention, release characteristics, antibacterial activity, indirect cytotoxicity, in vitro cell attachment, and cell proliferation of cellulose sponges incorporated with CMx/CS were investigated. As the results, the porous structure of CMx/CS-loaded cellulose sponges promoted a high ability to retain solution. In addition, the incorporation of CMx and CS improved the mechanical properties when compared to the neat cellulose sponges. Moreover, the addition of CS into the cellulose sponges showed inhibition against *E. coli* and *S. aureus*. Furthermore, the indirect cytotoxicity of the CMx/CS-loaded cellulose sponges was non-toxic and compatible with NCTC L929 and NHDF cells. Consequently, the CMx/CS-loaded cellulose sponge could be a good candidate for use as wound dressing materials.

Keywords: cellulose sponges, curcumin-β-cyclodextrin inclusion complex, chitosan, wound dressing, chronic wound

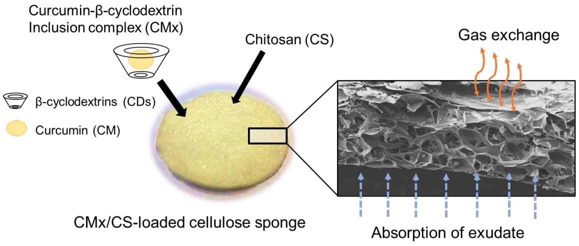

Figure 1: wound dressing based on cellulose sponge incorporated with curcumin-β-cyclodextrin inclusion complex

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pH-Responsive Dissociable Nanoscale Coordination Polymer for Diagnosis and Treatment of Atherosclerosis

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Abstract:
Atherosclerosis is a leading cause of death globally [1] due to the lack of early diagnosis and efficacious therapy. Here, a theranostic drug delivery system capable of T_1-weighted magnetic resonance imaging (MRI) [2] contrast and low-pH response to atherosclerotic plaque microenvironment is constructed. This theranostic system comprises nanoscale coordination polymers (NCPs) [3] developed by electronic interactions between acidic sensitive linker and gadolinium (Gd) ions, and a phospholipid bilayer modified on top of NCP to load simvastatin (ST). 1, 2-Distearoyl-sn-glycero-3-phosphoethanolamine-Poly(ethylene glycol) (DSPE-PEG) was integrated on the surface of the phospholipid bilayer to increase colloidal stability and extend blood circulation time. The resulting NCP-PEG theranostic system exhibits a well-defined "core-shell" structure at pH 7.4 to contain ST but collapses rapidly at pH 5.6 to achieve a marked release of ST *in vitro*. The theranostic system was evaluated *in vivo* with a high fat diet-induced atherosclerosis animal model generated using ApoE$^{-/-}$ male mice. Following intravenous administration, Cy5 fluorescence labeled NCP-PEG accumulated specifically in the established atherosclerotic plaques. Furthermore, MRI showed T_1-weighted signal was enhanced at the atherosclerotic plaque area after 24h intravenous injection (i.v.) of NCP-PEG. Therapeutically, intravenous administration of NCP-PEG/ST treatment once weekly for 8 consecutive weeks, at the concentration of 2 mg/kg attenuated atherosclerotic lesions compared to saline- and free ST-treated groups. In summary, we have developed a pH-responsive NCP-based nanoparticular system for concurrent MRI imaging and efficacious treatment of atherosclerosis in a preclinical model.

Keywords: atherosclerosis, nanoscale coordination polymers, magnetic resonance imaging, pH-responsive

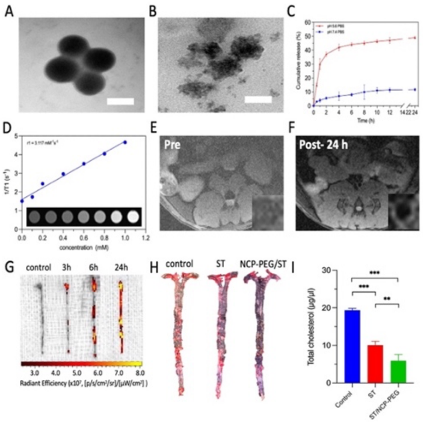

Figure 1: A, B) TEM images of NCP-PEG dispersed in PBS solution at pH 7.4 and pH 5.6, scale bar= 50nm. C) The cumulative release of ST from NCP-PEG/ST at pH 7.4 and pH 5.6. D) T_1 relaxation rate ($1/T_1$, s^{-1}) versus Gd concentration (from 0 to 1.2 mM). E, F) In vivo T_1-weighted MRI images of the aorta area. G) Ex vivo fluorescence images illustrating of Cy5 fluorescent signals in the aorta. H) Representative photographs of *en face* ORO-stained aortas from mice after different treatment. I) Serum level of total cholesterol.

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Posters

Synthesis and Characterization of Phenanthroimidazole Derivatives with Amphiphilic Chains

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Abstract:
Amphiphilic (hydrophilic and hydrophobic) molecular design is a viable strategy to achieve high degree of order at the supramolecular level, via sub nanometer phase segregation between hydrophobic and hydrophilic moieties, to ultimately modulate the properties of organic electronic materials.[1] Amphiphilic molecules with large π-conjugated cores have been employed to obtain excellent optoelectronic properties (e.g., charge transport, light emission etc.) associated with characteristic nanostructures[2]. The morphological control in the formation of the structures is an important topic and simultaneously still a challenge in the scientific research community. One versatile bottom-up method to fabricate materials on the micro- or nanoscale is the spontaneous self-assembly process.[3] The molecular system assembles spontaneously by intermolecular interactions to well-defined structures.

Here we report on the synthesis, crystal engineering and properties of amphiphilic phenanthroimidazole derivatives. Phenanthro[9,10-d]imidazole derivatives are recognized as efficient emissive and charge transporting materials for various applications related to organic electronics.[4]

The synthesized derivatives were characterized by ^{1}H and ^{13}C NMR, IR spectroscopy, mass spectrometry and single-crystal X-ray diffraction analysis. The thermal, optical, photophysical, electrochemical and photoelectrical properties of the materials will be reported.

Keywords: phenanthroimidazole, single-crystal diffraction analysis, self-assembly, OLED

Acknowledgements: This project has received funding from European Regional Development Fund (project No. 01.2.2-LMT-K-718-03-0019) under the grant agreement with the Research Council of Lithuania (LMTLT).

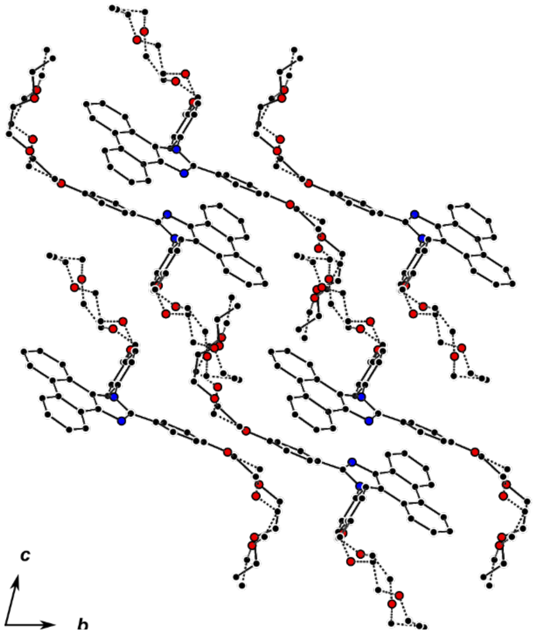

Figure 1: Projection of the (c,b)-plane of partially disordered model

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Production of self-assembled Ag nanoparticles in SiC matrix

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Abstract

We explore production of self-assembled Ag nanoparticles in SiC matrix by magnetron sputtering multilayer deposition. Different deposition temperatures and different multilayer compositions are used to obtain the self-assembling growth mode. In addition, the materials are annealed at different temperatures up to 500 °C after the deposition.

We show that the ordered lattice of Ag nanoparticles is already formed during the deposition at room temperature. Higher deposition temperatures lead to larger Ag nanoparticles. The investigated materials show the Ag surface plasmon resonance peak in optical properties, and its position and width depend on the deposition and annealing conditions.

Application of Cationic CNC and Nafion Membrane in the Electrolysis of Salt Solution

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Abstract:

The CNC separators obtained through the nanoization of cellulose in wood pulp have proven to be very valuable and are currently mainly used in composite materials for advanced functional applications. Among the nanocellulose materials, cellulose nanocrystals (CNC) are rigid rod-shaped crystalline particles with an aspect ratio (20-100).

A proton exchange membrane(PEM) such as nafion plays an essential role as the core of a fuel cell, and an excellent PEM has high proton conductivity, excellent mechanical strength, electrochemical stability, and satisfactory performance suitable for manufacturing MEMBRANE electrode assembly (MEA).

In this work, we applied the composite cationic membrane(sulfonated acid type cnc/nafion) in the electrolysis of salt solution. various membrane materials were prepared and tested to obt ain the caustic solution.

In the electrolysis of salt for the production of caustic soda, a semipermeable diaphragm membrane was used to separate the anode and catode compartments. with diaphragm cells, back migration of ions can be occurred, and is controlled by the rate of flow of fluid through the diaphragm. As well, that is also regulated by careful control of liquid levels. recently cationic non-porous polymer membrane is frequently used instead of diaphragm cell. the main purpose of polymer membrane such as nafion is to exclude OH- and Cl- ions from the anode chamber.

Keywords: Cellulose Nano Crystal, Cellulose, Membrane, PEM, MEA, Pulp, Sulfonated acid type cnc/nafion, Nafion membrane

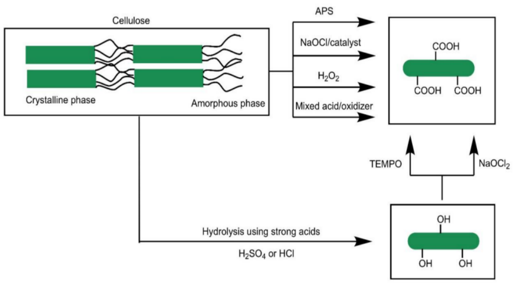

Figure 1. General methods for obtaining cCNCs from cellulosic sources.

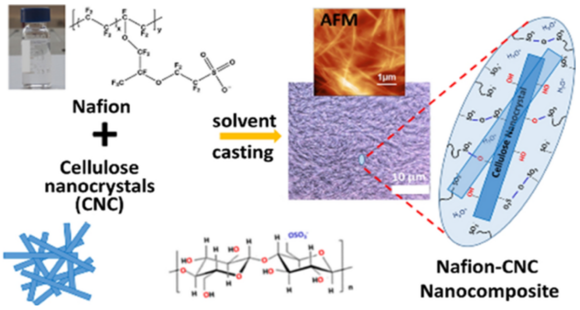

Figure 2. Mechanisms for synthesizing cnc and nafion

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Numerical studies of injection moulds for the production of bonded magnets

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Abstract:
The injection moulding process for bonded magnets fabrication has several advantages, namely allows the production of magnets with very complex geometries, high dimensional accuracy, mass-production, enables complex magnetization, e.g., multi-pole magnetization, and is suitable for hybrid processes, including fabrication of complex parts by overmoulding. Although a fraction of their composition will always remain as a non-magnetizable material, due to recent technical and scientific advances, this fraction is lowering, and bonded magnets are becoming stronger.

Nowadays, bonded magnets can be found in multiple applications across a wide variety of industries, such as the automotive industry, where they are used in electric drivers and sensor modules.

Concerning the magnetization process, permanent magnets or electromagnetic coils are typically incorporated in the mould to create a magnetic field in the cavity that magnetized the injected material.

In the present work, the main goal was to design a mould with permanent magnets to produce bonded magnets hard ferrite-based composites. Using numerical simulation, studies were performed to assess the impact on the cavity's magnetic field of different parameters: the mould materials magnetic properties, the magnets geometry and the location of the magnets at the mould. The best results were obtained for mould models conjugating two different classes of steel.

The Magnetized Gears project consortium is constituted by GLN Molds, the promoting company, and GLN Plast, CeNTI, PIEP and University of Minho as co-promoters. The project is co-financed by Portugal 2020, under the Operational Program for Competitiveness and Internationalization (COMPETE 2020), from European Regional Development Fund (ERDF).

Keywords: injection moulding, bonded magnets, numerical simulation

Strain-induced direct to indirect bandgap crossover in monolayer WSe$_2$

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Abstract:

Two-dimentional transition metal dichalcogenide (TMDC) materials, as direct-gap materials with strong light–matter interactions, have been the subject of recent interest. Recently, the strain engineering in the TMDCs employed the normal strain to modulate the band structures and intervalley couplings [1]. The normal strain changes the lattice constant and tilt the angle between bonds of the chalcogen atoms and transition metal atoms, altering the interaction between electronic states and thus modifying the electronic band structure. In this way, the lowest-lying K valley and Q valley in the band structure determine the optical bandgap, and change from direct-to-indirect (or indirect-to-direct) transition varying with the compressive strain. Here, the purpose of this work is to investigate the strain-induced direct-to-indirect bandgap crossover and its effects on photoluminescence (PL) and absorption charaeristics in monolayer WSe$_2$.

To verify the bandgap crossover, We traced absorption and photoluminescence (PL) under the externally applied strain as summarized in Fig. 1. Absorption peak near 1.7 eV was linearly varied from tensile to compressive strain. Meanwhile, PL peak energy near 1.7 eV was both blue-shifted under application of tensile strain while it was not considerably varied with compressive strain upto ~ -0.7% and followed by the spectral red-shift above -0.7%. The crossover from spectral blue-to-red shift of the PL peak energy can be well explained based on the band anti-crossing of the electronic orbital states under strain. We note that The Stoke shift of A exciton between PL and absorption was revealed with increasing compressive strain. The large Stoke shift is caused by the BAC-induced red shift in the PL spectra. Our results confirm strain-induced luminescence characteristcs and could provide a new route to straintronic device functionalization.

Keywords: photoluminesnce, strain, transition metal dichalcogenides, monolayer WSe$_2$, inter-valley coupling, band anti-crossing, Stoke shift

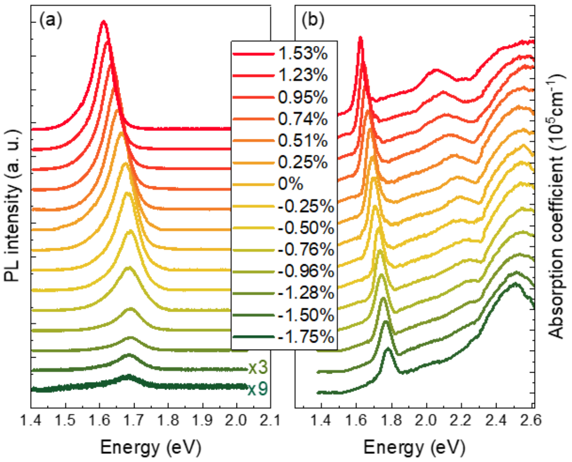

Figure 1: (a) PL intensity and (b) absorption coefficient spectra of monolayer WSe$_2$ as a function of strain. The black dotted arrows are the guide for eyes indicating the variation of A exciton peak energy.

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Low-temperature amorphous silicon deposition by DC sputtering

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Abstract:

Reactive sputtering is an excellent deposition technique for preparing compound films. High-purity films can be easily deposited by introducing a reactive gas into the chamber and sputtering the desired targets under a certain deposition conditions. A wide variety of metallic films, semiconductor layers, optical coatings, chemical sensors and opto-electronic devices have been deposited employing the reactive sputtering technique [1]. Reactive sputtering has several intrinsic advantages over other techniques like PECVD, such as low hydrogen content, lower cost, elimination of toxic gases and a much simpler deposition system. Moreover, characteristics including deposition rate and film composition can be controlled by the deposition parameters (substrate temperature, chamber pressure, reactive/non reactive gas flow, targets power, etc).

In the present study, we report the material properties of silicon thin films deposited by RF sputtering on three different substrates, Si(100), sapphire and GaN-on-sapphire templates, and under different deposition conditions. The samples were deposited using a pure (99.999%) Si target with an Ar (99.9999%) plasma with 2 sccm flow and a growth pressure of 0.47 Pa. Two sets of samples were developed: samples T20, T300 and T550 correspond to a deposition temperature of 20, 300 and 550 ºC, respectively; whereas P30, P40, P50 and P60 correspond to samples deposited with different DC power applied to the Si target, namely 30, 40, 50 and 60 W, respectively). In all cases a deposition time of 2 hours was used. Scanning electron microscopy (SEM) images of the samples indicate that a compact film grows on sapphire and Si(100) substrates regardless the deposition temperature or power applied to the target, even at room temperature. However, samples grown on GaN show a morphology made of thick nanocolumns. This change in the growth behaviour observed on GaN substrates can be attributed to different surface nucleation at the start of the process, which reduces the adatom mobility, and leads to thicker layers (Figure 1).

X-ray diffraction (XRD) data in 2θ/ω scan configuration do not show any peak associated with crystalline silicon (Figure 2). However, energy dispersive X-ray (EDX) measurements confirm the presence of silicon in the samples, so we can conclude that we are depositing an amorphous phase of silicon (a-Si).

We have demonstrated the possibility of depositing a-Si films on different substrates under different conditions. It should be noted that we could obtain compact a-Si films grown on sapphire and Si(100) even at room temperature. This opens the possibility of depositing on different kinds of substrate such as plastics for a wide variety of applications.

Keywords: Silicon, low temperature, DC sputtering.

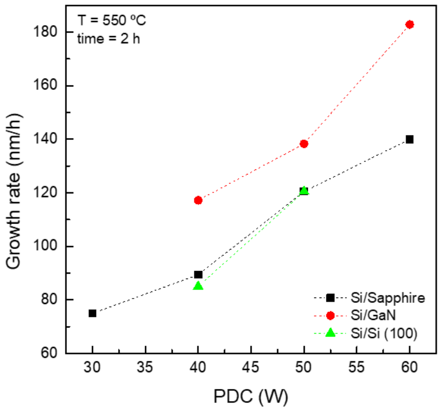

Figure 1: Growth rate of the Si layers as a function on the DC applied power and the type of substrate.

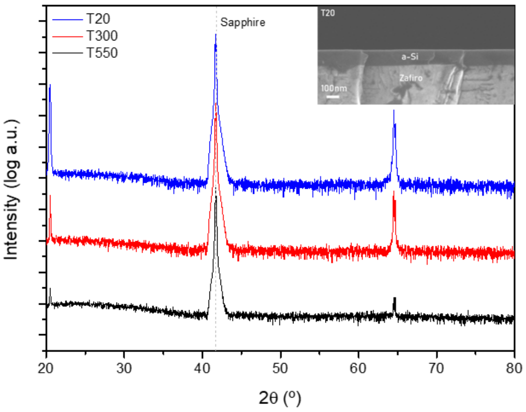

Figure 2: XRD data of Si samples deposited at different temperatures on sapphire. Inset: SEM image of a compact amorphous Si deposited on sapphire at 20ºC.

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Functionalization of Fiber Bragg Grating Using Different Coating Methods

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Abstract

Optical fiber gratings have gone through an improved growth of development in the current years in track with the observation of narrow band reflection in the photosensitive core region of silica optical fiber which is Germanium or boron doped. Fiber Bragg grating is a periodic modulation of the refractive index along the core of a photosensitive fiber. The refractive index changes are made by exposing the fiber to the interference pattern of Ultraviolet light. FBG's are less sensitive to refractive index (RI) variations of the external medium as the fiber is covered by cladding, limiting the application of FBGs being used in biological and chemical sensing applications. The surface of the e-FBG is modified with functionalized coatings based on the target to detect the change in RI using different coating techniques and different nanomaterial such as AgNP, AuNP etc. and is characterized. This sensing probe can be used in different biological sensing applications.

Keywords: Fiber Bragg grating, coating techniques, nanoparticles, functionalization,

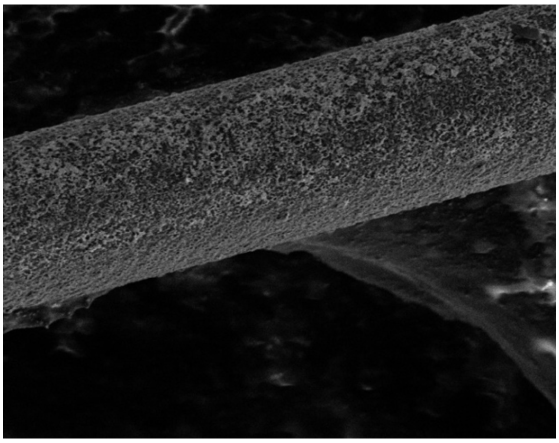

Figure 1: SEM image of etched FBG coated with gold nanoparticles using spin coating.

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Effect of Ag Doping on Threshold Switching Characteristics of Amorphous Ga_2Te_3 Film

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Abstract:
The memory devices with 3D cross-point array structure are attracting considerable attention due to the high density, simple structure, and applicapability to neuromorphic device. [1] However, due to leakage current occurring in unselected cells around the selected cell, operation failure can be occured. To address this leakage current, it is necessary to use a selector device that exhibits volatile threshold switching characteristics. [2] Several types of selector devices have been proposed, and among them, conductive bridge selectors are being actively studied due to their high selectivity and low off current. [3] In this study, the threshold switching characteristics of Ag-doped amorphous Ga_2Te_3 film were investigated. The T-plug shaped device was fabricated, as shown in Fig. 1. The Ag-doped Ga_2Te_3 film was deposited on the bottom electrode TiN film by using RF magnetron co-sputtering method. After the deposition of Ag-doped Ga_2Te_3 film, the top electrode TiN film was deposited by DC magnetron sputtering. The I-V curves of undoped and Ag-doped Ga_2Te_3 films are shown in Fig. 2. The undoped device showed ovonic threshold switching characteristics, including selectivity of 102 and leakage current of 4 µA. While, the Ag-doped Ga_2Te_3 film showed excellent threshold switching characteristics including high selectivity of 10^9 and low leakage current of 100 fA, as shown in Fig. 2. The Ag-doped Ga_2Te_3 devices are more advantageous for cross-point array memory applications due to their superior threshold switching characteristics compared to undoped devices.

Keywords: Cross-point array, threshold switching, chalcogenide, selector, sputter.

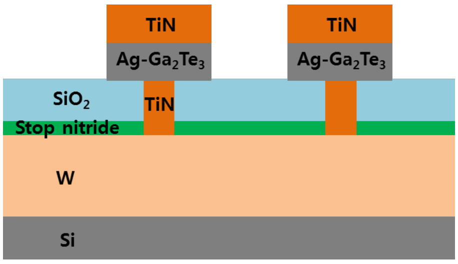

Figure 1: Schematic of the fabricated T-plug shaped device.

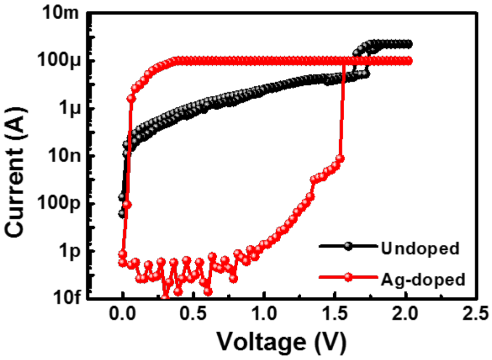

Figure 2: Measured I-V curves of undoped and Ag-doped Ga_2Te_3 selector devices.

Aknowledgement: This work was supported by the MOTIE (Ministry of Trade, Industry and Energy (project number 20010569)) and SK Hynix scholarship program.

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Exploring Bismuth Plasmonics In The Visible Spectrum

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Abstract:

Because Surface Plasmons (SP) are collective oscillations of electrons that propagate between the interface of a conductor and a dielectric [1], in the development of plasmonics the most used materials due to their high concentration of free electrons have been metals, in particular silver [2], gold [3] and aluminum [4].

In this work, we study the plasmonic response of systems formed by thin Bismuth (semimetal) films deposited on texturized substrates of porous anodic alumina denominated Bismuth metafilms (see Figure 1 a) and b)). Through reflectance measurements in the UV-Vis-NIR interval, we found dips in reflectance intensity, which we associate with Surface Plasmonic Resonances (SPR) of the first order [1], the SPR in the Bismuth metafilms can be excited and tuned to certain wavelengths varying the geometric parameters of the substrate.

We calculate the plasmonic response of Bismuth from reported experimental data of the dielectric function [5, 6], using an ideal theoretical model where the SPR are associated with the geometry of the system or the texture of the surface [7]. In this way, we observe that the curves calculated from the theoretical model reasonably follows the experimental data (see Figure 1 d)), nevertheless the last are mainly located above the calculated curves. We attribute the discrepancy; a shift of the experimental data to longer wavelengths, probably due to the dispersions produced by surface irregularities [8] and also possibly to the finiteness of the Bi films [9]. This tendency has also been observed in metafilms of other materials such as Al, Ag and Pb [10].

Although the free electron like Drude model for plasmonic response of Bi is located in the FIR region below ~0.03 eV [5], some experimental evidence indicates the existence of optical resonances in the UV-Vis-IR spectral range, which has been adjudicated to plasmonic resonances [11] and in our investigations we have demonstrated that SP can be excited in the near-UV-Vis-NIR range in Bismuth metafilms. This opens the possibility of studying the plasmonic properties of materials, not necessarily metallic, with the morphology of our metafilms.

Keywords: Bismuth, Plasmons, Metamaterials.

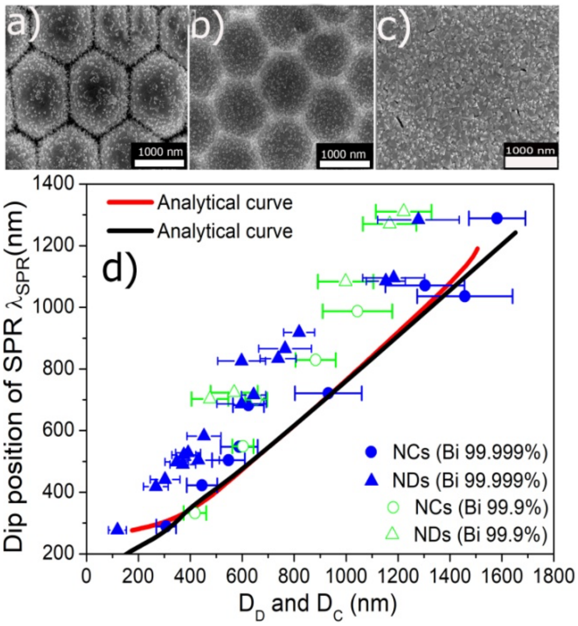

Figure 1: SEM images of Bismuth metafilms on two different types of substrates a) Nanodomes (NDs), b) Nanoconvaves (NCs), c) a film is shown on a non-textured substrate for comparison. d) Experimental data of Bismuth metafilms for Bi of 99.999% purity (closed blue triangles and circles) and Bi-MF of 99.9% purity (open green triangles and circles) and analytical curves calculated with the optical constants reported in [6] (red curve) and [5] (black curve).

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Applicability of low-cost FPGA boards in custom built Scanning Probe Microscopy electronics

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Abstract:
In this contribution we discuss different practical aspects of using low-cost Field-programmable gate array (FPGA) modules for performing complex control and data acquisition in custom built Scanning Probe Microscopes (SPM). While the use of a FPGA brings a potential for very fast data handling in custom built designs, it also has disadvantages, such as increased costs, complexity and a need for climbing a steep learning curve. Here, implementation and performance aspects of FPGA based boards in different types of control in the SPM will be discussed, including large area interferometric positioning systems for driving the XY scanner and feedback loop system for driving the Z scanner. Solutions for integrating the FPGA into data acquisition and data processing software tools will be demonstrated. Different data acquisition strategies for advanced SPM nanomechanical regimes will be discussed as well.

Keywords: Scanning Probe Microscopy, FPGA, data acquisition, interferometer, feedback loop, data processing, software.

Investigation of chemical reduction graphene oxide for supercapacitor application. Systematic research

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Michał Bielejewski[2], Paolo Samorì,[3]·Artur Ciesielski[1,3]

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Abstract:

Graphene is one of the most promising 2D material and it becomes central for many research fields including organic electronics, sensing, energy storage and conversion.[1] On the other hand, due to negligible amount of functional moieties which allow supramolecular interactions and covalent functionalization, the graphene oxide (GO) is more beneficial. Although, implementation of oxygen groups decreases of electrical properties such as: conductivity, capacitance, electron transfer in comparison with pristine graphene.[2, 3] To obtain material which combines electrical properties of graphene and ability for supramolecular interactions to occur, the chemically reduced graphene oxide (rGO) seems to be a great candidate. Therefore, rGO can be considered as good candidate for working electrical devices application. In this work we investigated and benchmarked several pathways of chemical reduction of graphene oxide to outline correlation between oxidation level and electrical properties of the material. The oxidation level was determined by C/O ratio which was estimated by X-ray photoelectron spectroscopy (XPS) and elemental analyses (EA). Electrical properties including specific capacitance and mechanism of energy storage have been studied by cyclic voltammetry, galvanostatic charge-discharge, electrochemical impedance spectroscopy and conductivity measurements. The various reducing agents such as L-ascorbic acid (AA), sodium borohydride ($NaBH_4$), hydrazine monohydrate (N_2H_4) and sodium hydrosulfite ($Na_2O_4S_2$) have been used. Moreover, the research investigates differences in structure, specific surface area, morphology etc. between 2 and 12 hours of reduction process. The influence of reductants on structural defects was confirmed by X-ray diffractions (XRD), Raman, infrared spectroscopy (IR) and solid state ^{13}C NMR characterizations. The results obtained from XRD and Raman measurement are presented on Figure 1. The most efficient reduction was achieved for sodium hydrosulfide while the highest level of oxygen species remained in case of $NaBH_4$ resulting in the lowest C/O ratio obtained from XPS. This study shows the possibility to obtain material with desired balance between oxygen content and electrical properties which allow to design materials for wide range of applications including energy storage systems, electrochemical sensors, field – effect transistors.

Keywords: graphene oxide, reduced graphene oxide, reductant, cyclic voltammetry measurements, capacitance, supercapacitors.

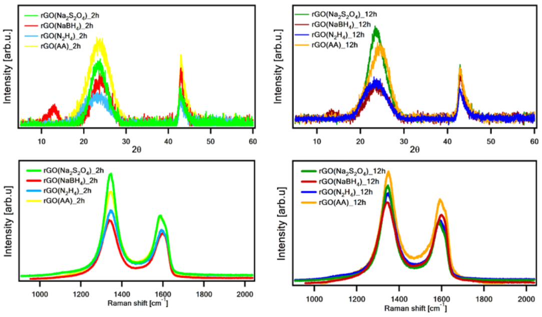

Figure 1: Figure illustrating the differences in XRD *(above)* and Raman *(below)* spectra between rGO obtained by various reducing agents and time of occurring reduction process.

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CNO-induced organization of well-defined star block polymers to obtain mesoporous carbon materials and their application in electrochemistry

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Abstract:

Porous carbon materials are abundantly applied in material science, especially in electrocatalysis or supercapacitors. Regular pore organization and narrow pore size distribution are crucial for the effective application of porous structures. These features can be obtained by involving well-defined copolymers consisting of *sacrificial* polymer blocks (polymer chains that undergo depolymerization during pyrolysis) and skeleton-forming polymer blocks, which transform into three-dimensional networks in the chemical or thermal processes protecting them from degradation in pyrolysis. Porosity and electrochemical performance can be enhanced by the incorporation of carbon nanostructures (*e.g.* carbon nano-onions (CNOs), carbon nanotubes) into the polymer matrix.

Herein, we report the synthesis of mesoporous carbon materials from novel polyacrylonitrile-derived diblock star polymers. Strict control over the size of the pores was obtained by shifting the length of the polymer blocks. Furthermore, the organization of polymers on the CNOs resulted in materials of higher surface area and superficial electrochemical performance.

Keywords: star polymer, RAFT polymerization, controlled polymerization, polyacrylonitrile, carbon nano-onions, pyrolysis, mesoporous carbon material

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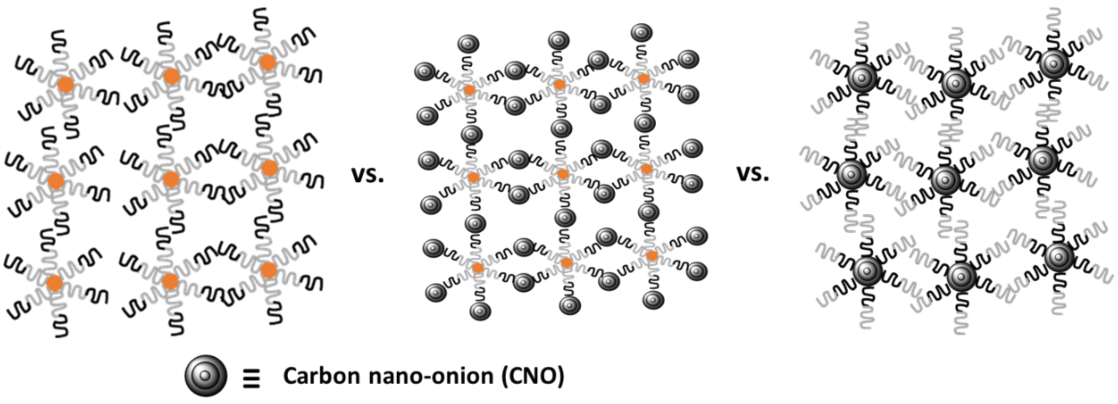

Figure 1: Figure illustrating the main goal of our research: does the organization induced by CNOs of defined polymers influences diameters of pores in polymer/CNOs hybrid matrix and pores in the carbon material derived from this matrix.

Synthesis of highly ordered carbonaceous materials with controlled formation of specific pore diameters and their application in electrochemistry and electrocatalysis

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Abstract:
The organization of specific pores in carbonaceous three-dimensional (3D) networks is crucial for efficient electrocatalytic processes and electrochemical performance. Larger pores, such as meso- and macropores, arise mainly from cross-linking of the oligomeric/polymeric chains in the presence of carbon nanostructures (CNs). The incorporation of CNs into polymers can create material structures that are more ordered compared to those of pristine polymers. Nanostructured hybrid materials used for energy conversion and storage employ block copolymers to control their morphology due to the copolymer soft-templating method. Strict control over the morphology of polymer chains can be achieved by reversible addition-fragmentation chain transfer (RAFT) polymerization.

In this study, we applied polymer-templated methods of carbon materials preparation, in which outer blocks of the star copolymers form the carbon skeleton, while the core part is pore-forming. Well-defined 6-*star*-(poly(methyl acrylate)-*b*-poly(4-acetoxystyrene)) dendrimers were synthesized by RAFT polymerization. They were then transformed into poly(4-vinyl phenol) derivatives subjected to polycondensation with formaldehyde and pyrolyzed at 800 °C. The selected star polymers were attached to carbon nano-onions (CNOs) to improve the organization of the polymer chains, resulting in higher porosity and better electrochemical performance of the resulting pyrolyzed hybrids. The physicochemical properties of all materials, including structure, morphology (Fig. 1), porosity, and electrochemical performance, were also investigated.

Keywords: carbon nano-onions, star polymers, RAFT polymerization, block polymerization, porous material, micro-and mesopores, specific surface area, supercapacitor, electrocatalysis.

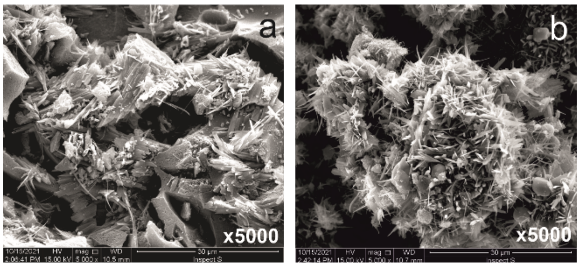

Figure 1: SEM images presented morphology of selected: (a) pyrolyzed star copolymer and (b) pyrolyzed CNO-polymer hybrid.

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Acknowledgment:
The authors would like to thank the National Science Centre, Poland, for its generous support of this work (grants: #2017/25/B/ST5/01414 and #2019/35/B/ST5/00572 to M.E.P-B).

Combined effect of multiple atomic interactions and structural catalysis on the H release from MgH_2 in Mg-Ni-rGO system

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Abstract:

Magnesium is a promising material in terms of hydrogen storage in the solid host for fuel cell application. However, its H release temperature is very high (>400 °C) at near ambient conditions. Normally, the H release kinetics of MgH_2 is improved using transition metal-based catalysts. However, such an improvement comes at a cost of gravimtric capacity in such a Mg system due to the heavy weight of the transition metals [1]. Therefore, light weight C-based materials such as graphite, CNT, activated carbon are used as catalysts for the H release from MgH_2 [2]. In the recent past, 10 wt.% rGO is added to MgH_2 which attenuated the delay in the H release (incubation) and improved the kinetics [3]. The synergetic effect of Ni and electrochemically exfoliated reduced graphene oxide (rGO) on the H uptake/release behavior of Mg is studied. Besides, the mechanism of hydrogen release was also analyzed experimentally. Addition of 3 at. % of Ni and 10 wt. % of rGO to Mg reduced the onset temperature of hydrogen release from MgH_2 to 275 °C. A high-energy ball milling of Mg, Ni, rGO establishes Mg-C and Ni-O-C interaction. These upon H uptake at 15 bar and 320 °C shows Ni-C and C-H interactions in XPS. The presence of Ni and rGO not only alleviates the incubation period but also shown superior kinetics compared to when they are added individually. The formation of the intermediate Mg_2NiH_x phase during the hydrogenation process shrinks the MgH_2 unit cell. This structural catalysis of the intermediate Mg_2NiH_x phase has further lowered the onset temperature of H release. The presence of multiple interactions and unit cell shrinkage leads to the formation of various local catalytic phases and catalytic junctions. This synergy of Ni and rGO help in releasing the hydrogen from the MgH_2 unit cell at a much lower temperature.

Keywords: MgH_2, rGO, Mg_2NiH_x, synergy, unit cell shrinkage.

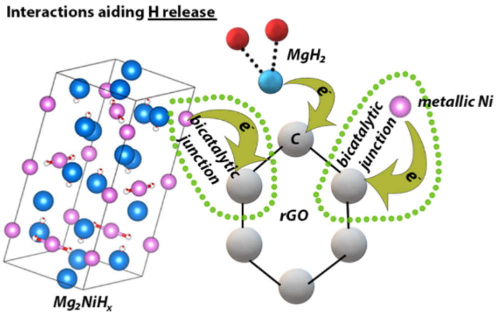

Figure 1: Figure illustrating the presence of multiple interactions which led to the formation of catalytic junction; these interactions expedite the reduction in the onset temperature of H release.

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Structural and dielectric properties of $CoFe_2O_4\backslash BaTiO_3$ Bilayers deposited over highly doped Si(001) substrates

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Abstract:

Nanostructured multiferroic thin films constructed by combining magnetostrictive and piezoelectric materials have attracted recently much scientific and technological interest [1]. In addition to possessing ferroelectricity and ferromagnetism in each individual phase, they are shown to exhibit stress mediated coupling between their magnetic and electric properties, called magnetoelectric effect. This coupling between their magnetic and electric degrees of freedom may then give rise to new physical phenomena and applications.

Barium titanate ($BaTiO_3$) is a ferroelectric material with good piezoelectric, pyroelectric and electro-optical properties which are favorable towards applications. Cobalt ferrite ($CoFe_2O_4$) presents a high magnetocrystalline anisotropy and magnetostriction, making it suitable for application in magnetoelectric composite thin films.

Here, bilayer composite thin films, composed by a $BaTiO_3$ (BTO) layer deposited over a $CoFe_2O_4$ (CFO) film have been prepared by laser ablation on higly doped conductive Si(001) substrates. Their structural, microstructural and dielectric properties were characterized. The X-ray diffraction and Raman spectroscopy measurements performed at room temperature show the presence of the tetragonal ferroelectric structure of $BaTiO_3$ and of the cubic spinel structure of $CoFe_2O_4$. The SEM micrographs show dense films, with cobalt ferrite and barium titanate layer thicknesses in the range 25nm and 140-420nm, respectively. Their dielectric properties were characterized by impedance spectroscopy. In order to obtain the relaxation times and activation energies, the electrical permittivity (figure 1) was fitted, using appropriate models [2] for the behavior of the polarization and including a conductivity contribution. As such, the influence of the synthesis conditions on the dielectric properties of the films and their evolution with individual layer thicknesses, will be discussed.

Keywords: Cobalt Ferrite, Barium Titanate, Multiferroic composites, Thin films, Laser Ablation, Structural properties, Morphology, Dielectric properties, Impedance spectroscopy

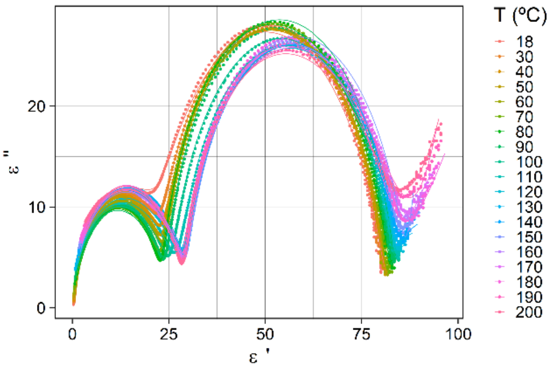

Figure 1: Nyquist plot, with the imaginary component of electrical permittivity as a function of real component, for the film with 25nm of $CoFe_2O_4$ and 140nm of $BaTiO_3$.

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Strong grain boundary non-radiative recombination peak around the angle (35°) of EBSD disorientation in CdSeTe thin-film Photovoltaics

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Abstract:
Cadmium Telluride (CdTe) solar cells are a very attractive thin-film photovoltaic technology because of low-cost manufacturing and high light absorption coefficient [1]. Electron hole pairs generated by photons absorbed in the solar cell have finite lifetime, due to radiative or non-radiative recombination processes. This has a harmful impact on solar cell efficiency [2]. One path towards increasing the efficiency of CdTe solar cells is to minimise non-radiative recombination at grain boundaries. This work aims to combine cathodoluminescence (CL) and Electron Backscatter Diffraction (EBSD) to investigate the effect of grain boundary disorientation on non-radiative recombination[3],[4]. An investigation between the non-radiative recombination and the grain disorientation in a CdSeTe solar cell has been carried out. EBSD images combined with CL Contrast, to determine the effect of grain boundary orientation on the recombination process. The CL intensity was high around 41° disorientation. This indicates that the non-radiative recombination is strong at this grain boundary disorientation. Also, CL intensity has small values at Coincidence Site Lattice (CSL) boundary which means the non-radiative recombination is low at this disorientation.

Keywords: CdSTe, Photovoltaic, solar cell,CdTe, interfaces, recombination, non-radiative recombination, grain boundaries, SEM, EBSD, CL, CSL.

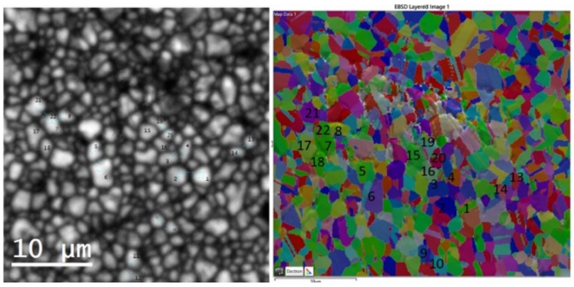

Figure 1: Figure showing CdSeTe a) panchromatic CL image, b)Electron backscatter diffraction map for the same picked grain.

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Nanostructured metal (Cr, Zr, Co) nitride thin film electrodes sputtered grown for excellent energy storage devices

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Abstract

Potential uses of transition metal nitride thin films have been envisaged based on properties such as higher conductivity than oxides, hardness, inertness and catalytic or electrochemical activity. Many current applications use nano-crystalline nitrides and their thin film based electrodes for excellent performance. Herein, we have deposited high quality thin films of transition metal nitride in controlled vacuum by using reactive dc- magnetron sputtering. DC magnetron sputtering is a process that provides an extremely efficient and highly flexible way of building coating architectures with varying degrees of complexity. In this work, we prepared highly crystalline and uniform thin films with good adhesion on flexible and conducting stainless steel (SS 304) current collector in Ar-N_2 atmosphere. Phase orientation, crystal structure and elemental composition was confirmed by XRD (X-ray diffraction) and XPS (X-ray photoelectron spectroscopy). Field Emission Scanning Electron Microscopy (FE-SEM) revealed the film thickness and morphology of the films, while composition was confirm by the EDAX attached with FE-SEM. Further, these deposited thin films of metal nitride were tested as an electrode material in aqueous solutions of 1 M Na_2SO_4 at various scan rates and current density. Electrochemical study of the electrodes was done by using Autolab PGSTAT302N.

Keyword: Transition Metal Nitride, sputtering, XPS, Cyclic Volumetric, Supercapacitor.

Ink-Jet Printed TiO_2 Thin Layers with Embedded Au Nanoparticles as Functional Layers for Perovskite Solar Cells

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Abstract:

Thin-film solar cells are of great interest due to the variety of methods for manufacturing functional layers, the possibility of using different types of substrates, and materials saving [1]. The weak point of thin-film solar cells is the lack of light absorption compared to a massive layer. One of the methods for capturing light is based on the introduction of metallic nanostructures in which a localized surface plasmon resonance (LSPR) can be excited [2]. In this work, a new strategy for deposition of thin TiO_2 layers with embedded gold nanoparticles (TiO_2/AuNP) is proposed. A way was developed for the synthesis of stable ready-to-print inks with complex gold nanoparticles synthesized by reduction from tetrachloroauric acid in the presence of TiO_2 nanoparticles and ethylene glycol [3]. The final formation of TiO_2/AuNP films occurred during the annealing of the layers, ink-jet printed on a substrate [4]. The size distribution of the gold nanoparticles forming on a substrate during drying and annealing depended on the ink storage time after the synthesis. The TiO_2/AuNP films demonstrated absorbance in the yellow-green range due to the LSPR. These layers are fully compatible with the electron transport TiO_2 layers of perovskite solar cells, deposited both by spin-coating or vacuum sputtering methods. The proposed strategy opens up new possibilities for modifying the architecture of perovskite solar cells by introducing LSPR structures. This is a promising approach to increase the efficiency of photovoltaic devices

Keywords: Gold nanoparticles, TiO_2, ethylene glycol, embedded, ink-jet printing, thin films, localized surface plasmon resonance, new methodology, efficiency, perovskite solar cells.

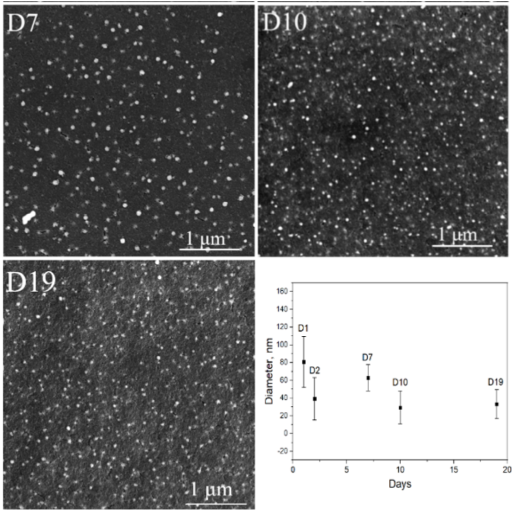

Figure 1: SEM images of the TiO2/AuNP films printed with the inks of different day-age and the day-age dependence of the size distribution of AuNPs in these films. The bars in the plot correspond to the standard deviation of the size. D7, D10 and D19 on subfigures correspond to 7-, 10-, and 19-day-aged inks.

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Development of a measurement method of voids in printed patterns to assess printability

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Abstract:

In printed electronics technology, the voids in the printed pattern could affect the quality of the patterns and consequently the performance of printed electronic devices[1]. Therefore, it is important to measure and control the voids in printed patterns during the manufacturing process. In this study, development of measurement method of voids in the printed patterns for international standard[2] was presented. The void has a three-dimensional shape and it is proper to measure the voids using a 3D microscope for accurate measurement. This study presented a measurement method for voids in printed patterns using a relatively inexpensive 2D microscope rather than expensive 3D microscope. In 2D image of printed patterns, pattern area and non-pattern area can be differentiated by brightness of the pixels constituting the image. Because of thickness variation and consequent brightness variation of pattern near void, the boundary differentiating void from pattern could be different depending on measurers when using 2D image. The proposed method introduced void threshold index as shown in Fig.1, ranging from 0 to 1 up to the measurer's choice, which defines the boundary between the void and pattern. Although the void threshold index is open to the measurer, and the size and area of measured void can be various(Fig.2), it was regulated that the measurer should report the value of void threshold index together with the measurement results for the reference of customers who would use the results in this international standard. The actual measurement results were presented to show the effect of threshold index on the measurement of voids(Fig.3). This cost-effective measurement method can offer simple and easy way to measure the voids and manage qualities of printed pattern for printed electronics industries.

Keywords: printed electronics, printed patterns, voids, printability, international standard.

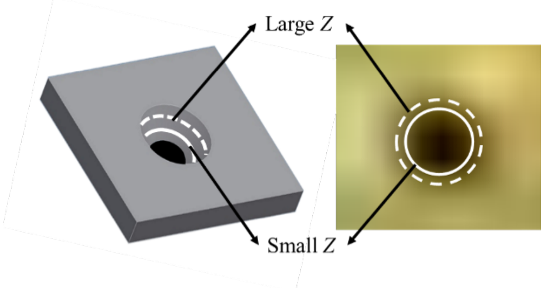

Figure 1: Effect void threshold index Z

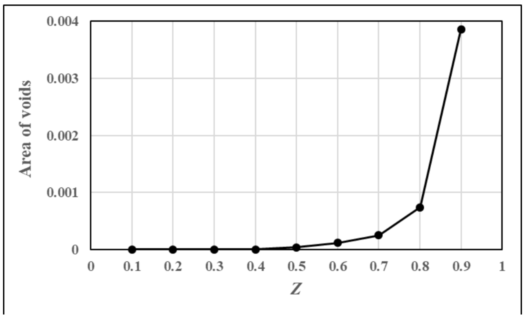

Figure 2: Dependence of area of voids on Z

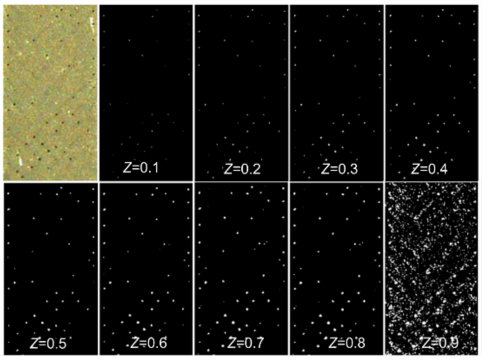

Figure 3: Binarized images of the same pattern with voids with varying Z

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Copper Silicide/SnSb Core-Shell Nanowires as a High-Capacity Material for Sodium-Ion Battery Anodes

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Abstract:
Alloying metals such as Sn and Sb have received received much attention recently as potential anode materials due to their high theoretical capacities and low cost. However, application of these materials has been limited due to pulverization caused by a large volume change that occurs during cycling. Nanostructuring the material is likely a key step in mitigating this issue as the nano-dimensions can accommodate the volume change without pulverization.[1] Forming composite materials of alloying metals is another method that has been successful in reducing pulverization. One such material is SnSb, which has been promoted as a promising anode material for sodium-ion batteries due to having a high theoretical capacity of ~750 mAh g^{-1} while reducing pulverization caued by volume change due to buffering that occurs between the metals.[2] Copper Silicide ($Cu_{15}Si_4$) nanowires (NWs) are a conductive 3D material that can act as a current collector for alloying materials such as SnSb without the need for binders, and have previously been suggested for use in Li-ion battery anodes.[3,4] In this work, we demonstrate the use of $Cu_{15}Si_4$/SnSb core-shell NW structures as a high capacity Na-ion anode material with potential for a long and stable cycle life. Using thermal evaporation, a nano-sized layer of SnSb is applied to the $Cu_{15}Si_4$ NW array to achieve a core-shell structure (Figure 1). The resulting 3D nanoarchitecture combines the benefits of nanostructuring and alloying composite materials in a single electrode. The large surface area of this structure and absence of binder allows higher mass loading to be achieved compared to planar or slurried variants of SnSb anodes.

Keywords: energy storage, sodium-ion battery, copper silicide, nanowires, alloying anode, low-cost battery, SnSb.

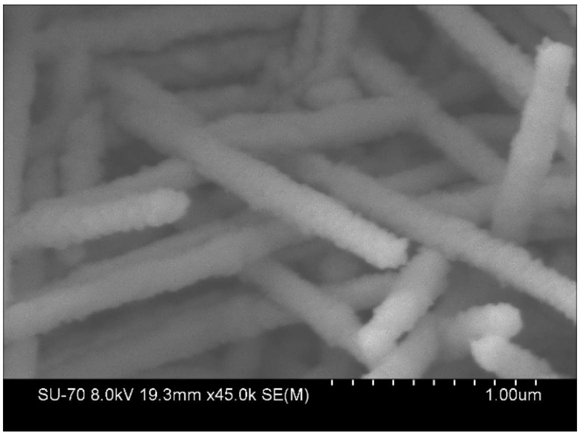

Figure 1: SnSb/$Cu_{15}Si_4$ NW structure imaged via SEM. Core $Cu_{15}Si_4$ NWs have a diameter of 130 nm and the SnSb coating has a thickness of 40 nm.

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Enhancing long-term photostability of $BiVO_4$/CdS photoanodes

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Abstract:

The development of cost-competitive materials capable of producing fuels or electricity directly from the energy harvested from sunlight offers a desirable approach towards fulfilling the need of clean energy. Recently, bismuth vanadate based photoanodes have attracted great amount of interest especially because of its narrow band gap energy between 2.4-2.5 eV, low cost and good stability. $BiVO_4$ is an n-type semiconductor and its use for solar water oxidation was first reported by Kudo et al. [1].

Nevertheless, $BiVO_4$ is disadvantages by its poor photogenerated charge carrier transport which leads to lower photocurrent density. We assembled CdS with $BiVO_4$ in order to obtain heterojunction formation and hence to achieve an even better photoelectrochemical response. However, the CdS suffers from photo-unstability which is its main drawback during the photo-illumination measurements. Then, CoO_x was loaded on the surface of CdS in order to improve both, PEC performance and stability [2]. The surface morphology images (Figure 1) were examined by Scanning Electron Microscope (SEM) and High Resolution Transmission Electron Microscope (HR-TEM). Observed from the SEM images BiOI are formed by very thin 2D plate-like nanosheats attached vertically to the FTO substrate which are after chemical and thermal treatment converted to round particles of $BiVO_4$. Fig. 1c demonstrates successful synthesis of $BiVO_4$/CdS heterostructure. The EDS elemental mapping reveals that CdS was homogeneously deposited on the surface of $BiVO_4$ while the CoO_x was randomly dispersed on the top that is usual for metal oxides serve as co-catalysts. To confirm the potential usage of the samples as photoanodes, the linear sweep voltammograms were measured. The current densities generated on bare $BiVO_4$ and CdS are 2.1 mA cm^{-2} and 1.9 mA cm^{-2}, respectively. Among them, current density of 4.54 mA cm^{-2} was obtained for $BiVO_4$/CdS which is more than two times higher than that of blank counterparts.

Keywords: semiconductor, $BiVO_4$, CdS, co-catalyst, photocatalysis, water splitting.

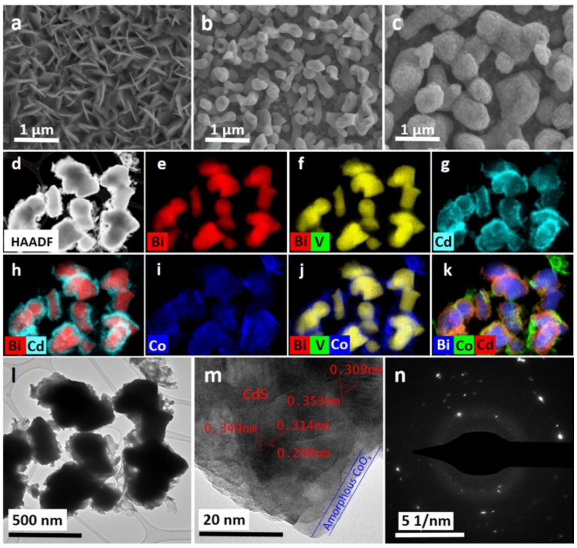

Figure 1: SEM images of (a) BiOI; (b) $BiVO_4$; (c) $BiVO_4$/CdS composite; (d) High-angle annular dark field (HAADF) image and (e-k) EDS elemental mapping of Bi, V, Cd, Co, joined Bi-V-Co and Bi-Co-Cd taken from $BiVO_4$/CdS/CoO_x composite; (l, m) HR-TEM images and (n) selected area electron diffraction pattern (SAED) of the as-prepared photoanode.

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Effect of experimentally verified nanofluid electrolytes to improve the electrochemical properties of flow batteries

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Abstract:

A study was conducted on the quantification of the kinematic viscosity, differential pressure and electrochemical properties of nanofluidic electrolytes to improve the performance of the application of vanadium oxidation/reduction flow batteries using aqueous electrolytes. The kinematic viscosity measurements for various nanoparticles and three nanofluids were compared with the theoretical formula, and in the case of nanoparticles having a hydrophilic functional group on the surface, it was confirmed that the kinematic viscosity characteristics were improved compared to the existing fluid at a relatively low content ratio. The differential pressure characteristics of the nanofluid for the porous carbon felt used as the VRFB active region were proportional to the nanoparticle content. The electrochemical performance measurement of the nanofluidic electrolyte was performed on MWCNT nanoparticles, and the oxidation/reduction peak current increased in proportion to the particle content in both the positive/negative electrolytes. In addition, in the case of the negative electrolyte, reversibility proportional to the nanoparticle content was confirmed.

Keywords: Nanofluidic electrolyte, Vanandium redox flow battery, Kinematic viscosity

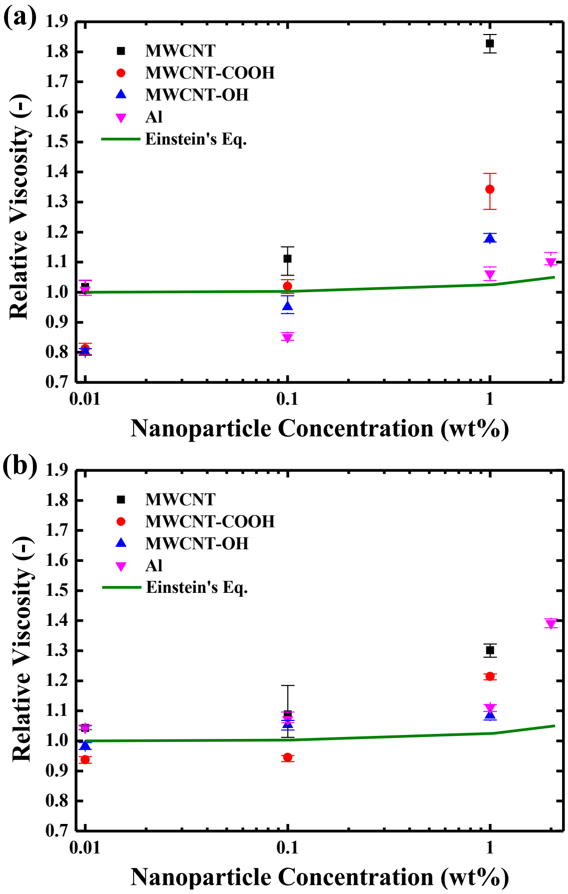

Figure 1: Relative kinematic viscosity of nanofluids; Base-fluid (a) positive VRFB electrolyte, (b) negative VRFB electrolyte.

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Ultrafast laser-based fabrication of Efficient Anti-reflective Silicon Nitride nano/microstructures for Optoelectronics applications

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Abstract:

It is vital to enhance solar cell efficiency in order for photovoltaic power generation to be a realistic alternative to the global energy challenge. Enhancing the amount of sunlight that reaches the photo-conversion layer is one approach that could be taken. To pattern Silicon Nitride (SiNx), various techniques have been developed, such as photolithography with wet etching in acidic solutions [1]. However, this method necessitates a number of process steps, as well as costly equipment and toxic chemicals. To fabricate fine structures with well-defined edges on SiNx thin films, a nonlithographic or direct patterning strategy must be developed. Laser ablation is the expulsion of materials from a substrate by direct absorption of laser energy, which can yield the required combination of narrow and clean patterning due to their advantage in regionalized heating and material expulsion. Research teams studied the interaction of femtosecond laser pulses with various materials such as silicon, Al, and ITO in the presence of air, water, and sulfur hexafluoride (SF6) [2]. The current work reveals the fabrication of nanostructures on SiNx over silicon substrates using femtosecond laser writing in an air medium as shown in Figure 1. These micro/nanostructures have a diameter of about 300-400 nm and resemble structures. It has discovered that micro/nanostructures structures form as a result of the interaction of femtosecond pulse-induced plasma with a SiNx/Si substrate. The absorption of intense light in a thin SiNx/silicon layer produces a plasma at the SiNx-air interface. The plasma then equilibrates with the surrounding air and SiNx, resulting in a layer of molten silicon on the surface. Furthermore, these fabricated structures have been characterized using scanning electron microscopy (SEM), Raman spectroscopy, crosssection FESEM, and a UV-VIS spectrophotometer for optoelectronics applications such as Photovoltaic and Surface Enhanced Raman Spectroscopy (SERS). In the wavelength ranges of 400–800 nm, and 200-1000 nm, respectively, average specular reflectance of 2.82 percent, and 5% are attained, with an average absorptance of 95 percent within 0.2–1 µm. The material easiness, patterning versatility, boosting capability, structural reliability, and self-cleaning quality can meet the necessary criteria for useful light-harvesting applications.

Keywords: silicon nitride, femtosecond laser, laser texturing, Laser-matter ablation, surface chemical processing, Nano/microstructures, micropatterning, photovoltaic applications.

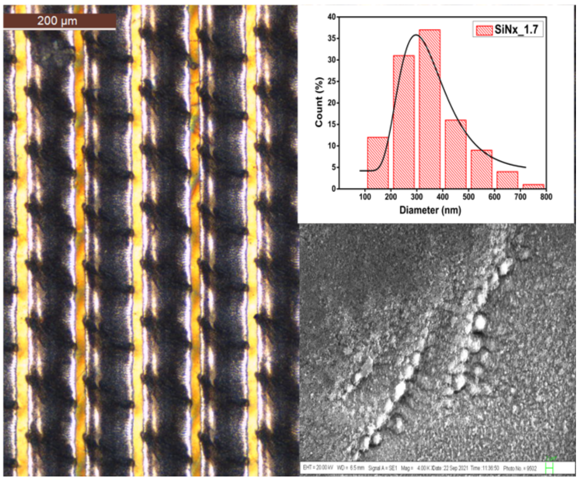

Figure 1: Figure illustrating the optical microscope photograph of femtosecond laser patterned SiNx has a refractive index of 1.7 on Si substrate. The inset figure shows Nano/microstructures fabricated along with their particle size distribution histogram indicating 300-400nm diameter after laser texturing.

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In-silico design of graphene plasmonic hot-spots

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Abstract:

Plasmons are able to confine light down to the nanometer scale and, in turn, to produce an enhancement of the electric field under the effect of an external electromagnetic radiation.[1]

Single molecule detection becomes possible when huge enhancements arise in very precise region of space (i.e. hot spost).[2] Such a confinement is usually obtained by exploiting specific geometrical arrangements of plasmonic substrates, like metal nanoparticles (MNPs).[2]

However, such behavior has not been confirmed for graphene nanostructures, although graphene shows extraordinary optical properties due to the formation of highly localized surface plasmons.[3]

In fact, pristine graphene has been used as a substrate for the so-called Graphene Enhancement Raman Scattering (GERS), but the measured enhancement in the molecular Raman signal is orders of magnitude lower than for MNPs.[4] Therefore, the use of graphene as plasmonic substrate for single molecule detection is being hampered by its low enhancement factors.

In this contribution, we propose a computationally driven design of geometrical arrangements, specifically engineered to maximize the field enhancement in graphene-based nanostructures. Our approach is based on a fully atomistic approach that we have recently developed.[5,6]

In particular, we focus on the enhancements effects arising close to edge defects and grain boundaries in polycristalline graphene (PCG), which are usually present in graphene samples (see Figure 1). Also, we consider geometries inspired by nanocavities allowing single molecule detection on metal substrates.[1]

In all test cases, the enhancement factors are comparable to noble metal substrates due to the creation of localized nanocavities, thus potentially paving the way for single molecule detection from graphene-based substrates.

This work has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (grant agreement No. 818064).

Keywords: ωFQ, atomistic model, graphene, plasmonics, defects, grain boundaries, hot spots, optical spectra, electric field enhancement, nanocavity.

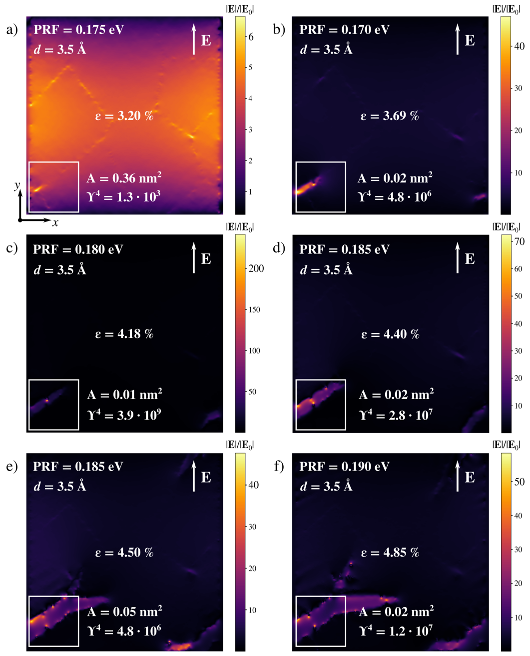

Figure 1: Computed $|E|/|E_0|$ color maps of PCG under isotropic strain ε = 3.20 % (a), 3.69 % (b), 4.18 % (c), 4.40 % (d), 4.50 % (e) and 4.85 % (f), at E_F = 0.4 eV. The maximum enhancement is computed in the region highlighted in the white box.

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CuInS/ZnS Core-Shell Quantum Dots A Green Alternative to Cd and Pb Core-Shell Quantum Dots

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Abstract:

The tunability of optical and electrical properties of core-shell quantum dots (QDs) is highly desirable in photovoltaic devices. Core-shell quantum dots have been simulated and demonstrated in recent years to have excellent optoelectronic properties. Depending on the radius of the core and thickness of the shell, the charge carrier behavior can change form type I (electrons and holes are confined in the core), type II (electrons and holes are separated into core and shell regions), to quasi-type II (one type of charge carrier is localized in the core or shell while the other type of charge carrier is delocalized). In addition to charge carrier behavior, the optical emission can be tuned by controlling the radii of the core and shell. Currently, most of the studies reported have been limited to Cd and Pb based QDs [1,2,3,4]. Cd and Pb are commonly known to be carcinogenic elements, which limits the applicability of the particles. Alternatively, Cu and In based QDs have been reported to be biocompatible [5]. This can open the applicability of core-shell QDs beyond photovoltaic systems to potential biomedical applications. Herein, we explore the optoelectronic properties of CuInS/ZnS QDs synthesized at low temperature with polar ligands [6]. We observed size tunability of the core by taking samples at different time intervals (Fig. 1.A). The size tunability is indicated by a redshift of the emission peak as the reaction time increases. Modifying Cu to In ratios, we have observed that there is an optimal compositional ratio that maximizes the photoluminescent quantum yield (Fig. 1.B). The photoluminescence was enhanced by the addition of a ZnS shell. Fig. 2 shows the Stokes shift between the absorption and emission spectra of CuInS/ZnS QDs. The optical bandgap was studied by applying Jarosinski and Pawlak Inverse logarithmic derivative method (ILD) to the absorption spectrum [7], indicating an indirect bandgap. The results were compared to Tauc's method. Our preliminary experimental observations suggest that Cu and In based QDs may be an alternative replacement for Cd and Pb based QDs.

Keywords: Polar Quantum Dots, Core-Shell, ILD Method, Cd Pb Free QDs

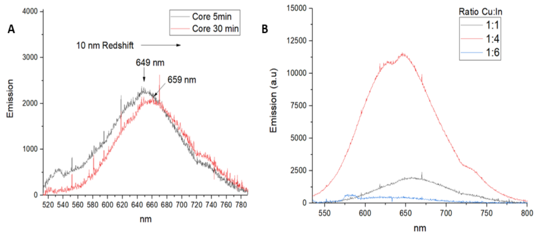

Figure 1: A) Photoluminescence spectra of CuInS QDs core at different reaction times. excited at 450nm B) Photoluminescence of CuInS/ZnS with different core compositions excited at 450 nm.

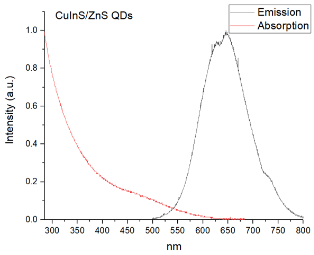

Figure 2: Absorption and emission spectra of CuInS/ZnS QDs.

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Advancements in white electroluminescent carbon dot- based light emitting diodes

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Abstract:

Photoluminescent carbon dots or carbon “quantum” dots have emerged as a new class of brightly fluorescent nanomaterials for biological, sensing, and optoelectronic application since their first synthesis. [1,2,3,4]
In this presentation, we show a new multilayer configuration of an electroluminescent LED structure (ITO/HIL/HTL/CDs/Al) of the functionalized carbon-dots-based white light-emitting device (CD-WLED) (Fig.1)

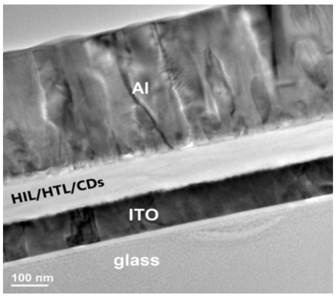

Figure 1: TEM image of the multilayer structure of ITO/HIL/HTL/CDs/Al CD-WLED

The LED structure, with the carbon dots layer sandwiched between the hole transport layer and the low-work function Al cathode, was evaluated by applying a forward bias on the hole-injecting contact. The corresponding electroluminescence (EL) was found to be broad, covering a wide range of the visible spectral region (Fig.2a) with an increase in intensity as the applied current increases from 50 to 100 mA. The comparison of the EL and the collection of multiple photoluminescence spectra presented in Fig.2b suggests that the recombination zone is within the CDs layer.

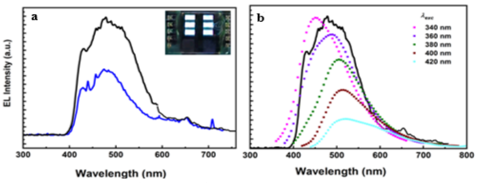

Figure 2: a) Electroluminescence at 9V applied bias and current of 50 mA and 100 mA (Inset: photo of the CD-WLED); b) EL (solid line) and PL spectra of the solution-based carbon dots at indicated excitation wavelengths (dash lines).

Keywords: carbon dots, CW-LED, electroluminescence, white LED.

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Phenothiazinyl-substituted Bis(trifluoromethyl)biphenyl Compound for Efficient Oxygen Sensing

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Abstract:

Biluminescence, or dual-state emission, refers to compounds which are able to exhibit fluorescence and phosphorescence simultaneously.[1] Dual-state emitters have attracted a great deal of attention recently due to their wide potential application range including oxygen sensing in biomedical applications anticounterfeiting, delayed electroluminescence, etc.[2] For efficient dual-state emission, strong spin-orbit coupling is necessary to ensure proper intersystem crossing (ISC) from singlet to triplet excited state as well as efficient room temperature phosphorescence (RTP).[3] In order to favour the ISC process, specific design strategy of pure organic RTP molecules has to be employed, e.g., incorporation on heavy atoms, such as Br, I, Cl; bulky moieties, such as benzoyl group; or choice of highly symmetrical planar aromatic fragments.[4]

In this work, compound containing phenothiazine donor moieties exhibiting dual-state emission in blue-green region will be presented. Phenothiazinyl-disubstituted bis(trifluoromethyl)biphenyl was found to be a highly sensitive and fast-responsive oxygen sensing compound with the highest sensitivity reported so far. The experimental results will be supported by theoretical study of molecular design and electronic transitions of dual-emissive material.

Keywords: dual state emission; room temperature phosphorescence; phenothiazine; biphenyl.

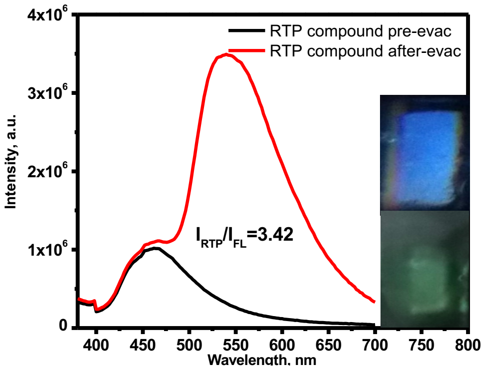

Figure 1: Photoluminescence spectra of 10% solid solutions of RTp compound in Zeonex recorded at room temperatures (Insert: emission changes of the sample of compound 4 molecularly dispersed in Zeonex).

Acknowledgment: This research has received funding from European Social Fund (project No 09.3.3-LMT-K-712-19-0033) under grant agreement with the Research Council of Lithuania (LMTLT).

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Advanced materials based on azulene-phenyloxazolone

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Abstract:
New azulene phenyloxazolones [1] were electrochemically investigated by cyclic voltammetry, rotating disk electrode and pulse-differential voltammetry in 0.1M TBAP / CH_3CN (Figure 1). Chemically modified electrodes (CMEs) based on these ligands have been synthetized and tested by ferrocene redox probe, electrochemical impedance spectroscopy, AFM, SEM using approaches similar to those recently published for other azulene derivatives [2]. The obtained CMEs were compared and tested in the detection of heavy metal (HM) ions [3]. The influence of the preparation conditions (charge and potential) has been examined for CMEs obtained using different ligands. The CMEs were finally used for the analysis of synthetic samples of HMs. In addition, an *in silico* study on the optimized geometries of the studied ligands were carried out in order to reveal important paramters for assessement of their electrochemical behaviour. Variation of computed properties related to electronic density and charge distribution, obtained using DFT/B3LYP/6-31G* functional method [4, 5], has been analyzed in terms of azulene substitution (Figure 2).

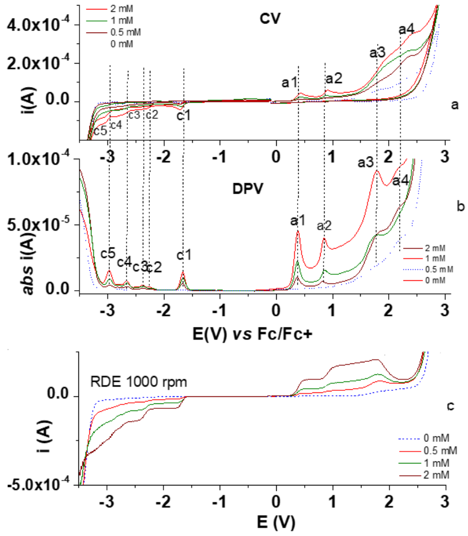

Figure 1: CV (a), DPV (b), and RDE (c) curves for different concentrations of azulene-phenyloxazolone C (1 mM in 0.1M TBAP / CH_3CN).

Keywords: azulene-phenyloxazol-5(4H)-ones, AFM, SEM, EIS, quantum chemical reactivity parameters, HMs analysis.

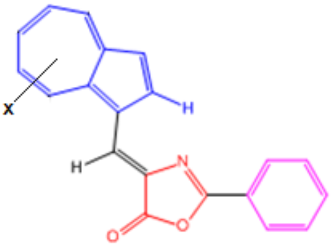

Figure 2: Investigated azulenes; X = H (A), 4,6,8-trimethyl (B), 5-isopropyl-3,8-dimethyl (C).

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Synthesis and repetitive application of nanocrystalline ZnO based floating photocatalyst for the detoxification of water from bacteria and viruses mixtures

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Abstract:
Photocatalytic treatment of contaminated water by UV or visible light irradiated ZnO, TiO_2, and some other semiconductor materials is recognized as a highly promising universal and environmentally friendly detoxification method [1]. However, usually the most efficient photocatalyst materials are synthesized as fine nanocrystalline powders and this rises significant handling and repetitive application issues. More recently, researchers started to immobilize photocatalyst (nano)materials on relatively large low density supports creating floating photocatalyst particles or grains [2]. Such approach allows to effectively retrieve the used photocatalyst material and to reapply it for the treatment of new portion of contaminated water. While TiO_2 based floating photocatalysts were synthesized and tested by relatively large number of researchers, the reports on ZnO based floating photocatalysts remain scarce. Especially, there very limited information on how ZnO based photocatalysts can deal with the water detoxification from biological contaminants like bacteria, viruses and their mixtures. Accordingly, in current study we used reactive magnetron sputtering technique and deposited unconventional orange color nanocrystalline ZnO based photocatalyst on borosilicate glass and floating high-density polyethylene (HDPE) grains. The structure of the synthesized photocatalyst was characterized by XRD, SEM, and XPS techniques. The supporting repetitive measurements of the ZnO based photocatalyst film efficiency under visible (estimated by dye bleaching tests) showed high stability over ten cycles. Visible light induced photocatalytic efficiency of the floating photocatalyst grains (FPG) was estimated by repetitive treatment of water samples containing *Salmonella typhimurium* (strain SL1344) and *Micrococcus luteus* bacteria, as well as water samples containing PRD1 and T4 bacteriophages (viruses that infects bacteria). The repetitive photocatalytic treatment tests indicated complex interaction between the bacteria, viruses, photocatalyst and its HDPE support. But primarily they revealed that FPGs lose most of its photocatalytic efficiency in just 3 cycles. In order to stabilize the ZnO based FPGs and enhance its photocatalytic efficiency under the visible light, before the depositing ZnO films we pre-covered HDPE grains by Ni underlayer. The addition of Ni resulted in mixed results. For example, this reduced the efficiency S. typhimurium disinfection during the first cycles, but increased the detoxication stability over consecutive tests (Fig. 1).

Keywords: ZnO, floating photocatalysis, nanomaterials, magnetron sputtering, photocatalytic disinfection, environment.

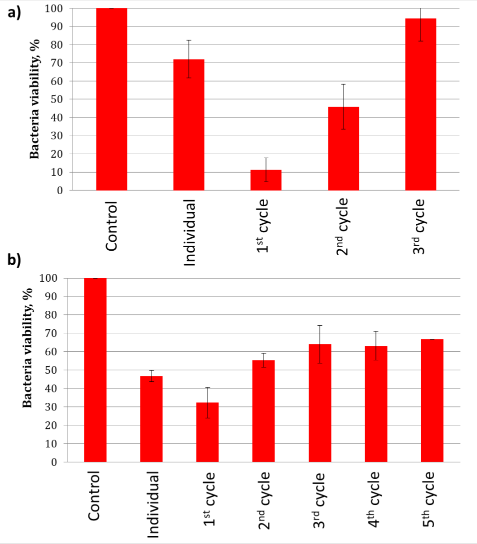

Figure 1: The efficiency of *Salmonella typhimurium* bacteria disinfection in water: a) treatment performed using ZnO based floating photocatalyst grains without Ni underlayer; b) with Ni underlayer.

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Ivestigation of bi-layered ZnO-Ni photocatalyst powder produced by reactive magnetron sputtering technique

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Abstract:

Generaly, different synthesis methods produce photocatalyst material with different merits. Sol-gel and other chemical methods commonly produce nanocrystalline powder, which typically has very large surface area [1]. Meanwhile, magnetron sputtering and other physical methods usually deposit films and benefit from more defined control of the photocatalyst structure formation and is a more convenient way to form heterostructures [2]. On the other hand, these methods most often can not provide such high surface area and product output as chemical alternatives. To evade these limitation, the goal of the current study was to use the magnetron sputter deposition method in non-conventional way and to produce bi-layered ZnO-Ni photocatalyst powder with enhanced functionality. To synthese such bi-layered powder, at first magnetron sputtering was used to deposit thin Ni layer on NaCl grains. Then reactive magnetron sputtering was used to deposit ZnO layer on top of the pre-coated salt. After Ni and ZnO deposition (schematic view is presented at Figure 1a), coated salt grains were poured into distilled water to dissolve NaCl. SEM and EDS analysis (Figure 1b and 1c respectively) of washed and dried loosed bi-layered ZnO-Ni particles revealed that they can be characterized as open shells with Ni on one side and ZnO on the other side. The corresponding composition and structure of the particles was also confirmed by XRD and XPS methods. The key purpose of Ni side was to supplement the ZnO photocatalyst powder particles with the magnetic properties and to make them responsive to the magnetic field. Such feature of the photocatalyst powder particles was foreseen to be very useful for the repetitive photocatalytic water treatment. Indeed, in laboratory tests, the concept worked swimmingly and most part of the initial bilayered powder were sucesfully recolected after 10 consequetive collect-release cycles. The photocatalytic activity of the bilayered ZnO-Ni powders was estimated by the bleaching of dyes under UV and visible light. Also, powders were used for the photocatalytic treatment of *S.Typhimurium* bacteria. In these tests, powder effect for the bacteria viability, cell membrane pemeability and bacteria sensitivity to the antibiotics were determined.

Keywords: ZnO, Ni, photocatalysis, photocatalyst, bi-layered nanomaterials, reactive magnetron sputtering, photocatalytic bleaching, ferromagnetic coatings, water technologies, environment.

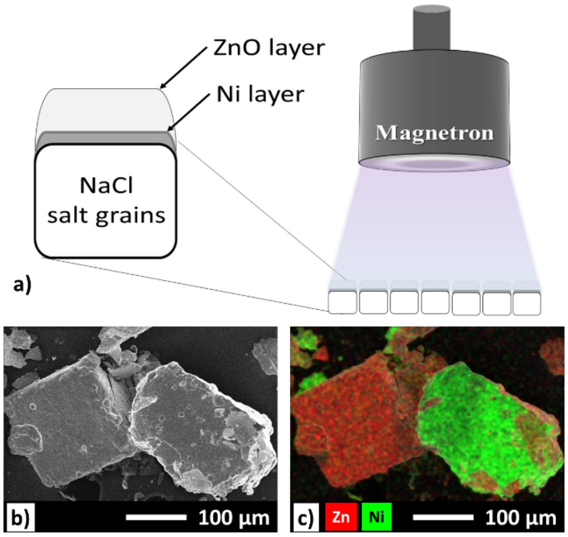

Figure 1: Experimental scheme of the bi-layered ZnO-Ni photocatalyst particles formation on NaCl grains (a), SEM image of ZnO-Ni photocatalyst particles showing external side (left) and internal (right) sides of the "shells" (b), EDS elemental mapping image of Zn (red dots) and Ni (green dots) (c).

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Reduced graphene oxide/gold nanoparticles nanocatalyst: Applications for Suzuki reactions in water and oxidative esterifications

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Abstract:
Carboxylic acid derivatives are one of the important building blocks and widely used in pharmaceuticals, polymers and natural products synthesis. Among the available synthetic methods, an effective route has been developed via oxidative esterification of the achievable aldehydes or alcohols. However, some of these procedures require the use of stoichiometric amounts of heavy-metal oxidants. Thus, it is significant to find sustainable benign reactions conditions for the oxidative esterification of aldehydes. The protocol of structurally integrated gold metal is expected to offer tremendous prospects toward emerging functions of graphene-based nanomaterials. In our research, gold nanoparticles dispersed on reduced graphene oxide (Au/rGO) were prepared *via* reduction of gold (III) complex using sodium citrate. The prepared Au/rGO is composed of well-defined reduced graphene oxide support decorated with gold nanoparticles (10-13 nm). The chemical, morphological, and size analyses of Au/rGO by XRD, XPS, TEM/HRTEM/EDS, AAS, and Raman spectroscopy revealed that the hybrid material is possessed of a well-defined rGO support decorated with gold nanoparticles. The efficiency of catalyst was evaluated for Suzuki-Miyaura coupling reactions in water and oxidative esterification of aldehydes under ambient condition using environmentally friendly oxygen as an oxidant (Figure 1). The catalyst displayed high activity and found to be significantly reusable with elimination of toxic organic solvents and expensive ligands.

Keywords: gold nanoparticles/reduced graphene oxide, oxidation reactions, heterogeneous catalysis, sustainable protocol

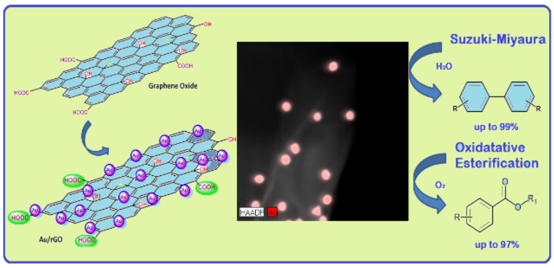

Figure 1: Gold nanoparticles dispersed on reduced graphene oxide (Au/rGO) were prepared *via* reduction of gold (III) complex and used for Suzuki-Miyaura reaction and oxidative esterification reactions under benign conditions to obtained excellent yields.

References:

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Immobilized functionalized silver nanoparticles to detect Chromium in water.

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Abstract:

A simple yet effective way to detect chromium, one of the major water contaminant by using Tartaric acid functionalized silver nano particle immobilized on the surface of etched Fiber – Bragg grating sensors (e-FBG). The target analyte and functionalized nano particle could be further confirmed by performing UV-Visible spectroscopic analysis while the structure of the coating surface could be analyzed by SEM imaging.figure 1 provides an insight into the working principle of the devolped sensor.The limit of detection(LOD) falls well with in the permissible range. The sensitivity and linearity of the sensor shows promising signs of developing into a field deployable unit.

Keywords: Chromium detection, silver nao particle,functionalization, e-FBG.

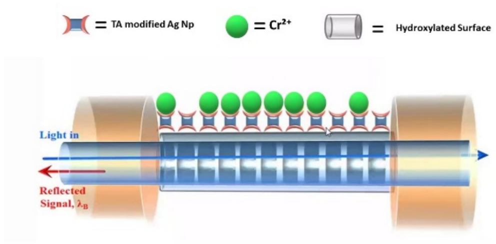

Figure 1: Figure illustrating the fundamental-Working principle used for sensing Chromium in water sample, using nano material coated e-FBG sensor .

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The Possibility of Reactive Printing on Inherent Flame Retardant Fabrics

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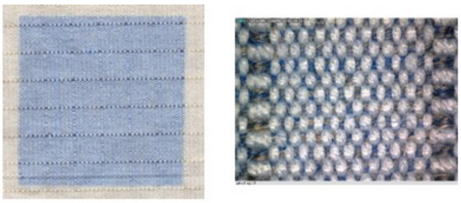
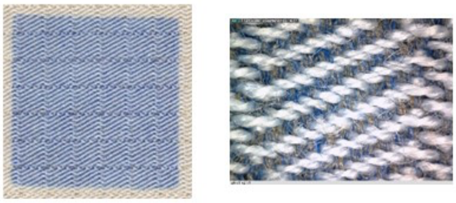
Abstract:
The complexity of the composition of inherently flame retardant fabrics makes it difficult to treat them in dyeing and printing procedures, and it is extremely difficult to achieve a certain aesthetic component of such fabrics. In this research, the analysis was performed on three selected types of inherent flame retardant fabrics whose composition and construction was designed at the University of Zagreb, Faculty of Textile Technology as part of a project for the development of fire retardant fabrics for dual use. The warp and weft composition of the tested fabrics are as follows: warp: 95% m-AR; 5% para-AR; weft: 30% PA 6.6; 35% m-AR; 35% CV FR. The three fabric samples differ in structural characteristics: Fabric 1 is weaved in reps, Fabric 2 in twill 2/2, Fabric 3 in twill 3/1. The samples were subjected to a process of printing with reactive dyes, applying two concentrations of dyestuff and two types of thickeners each in two viscosities achieved with different ratios of dry matter and water. The samples were tested for flame retardancy by determining the Limited Oxygen Index (LOI), and the analysis of the print quality was performed by the test of wash fastness and colorimetric evaluation of the printed areas before and after washing. The achieved colour strength was analyzed through the objective evaluation of K/S values. The colouration of individual fabric components was analyzed by microscopic imaging of printed surfaces. The research is related to the development of a functional fabric that has the properties of inherent non-flammability and high comfort whose visual and functional properties can be improved through printing.

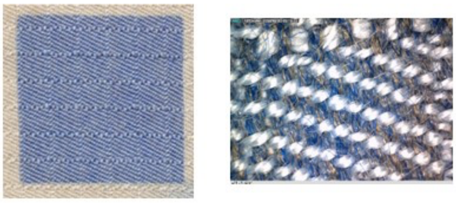
Keywords: textiles, flame retardancy, printing, reactive dyestuff, aramid, CV FR, spectrophotometry, wash fastness, microscopic imaging.



Fabric 1



Fabric 2



Fabric 3

Figure 1: The figure shows the prints of samples Fabric1, Fabric 2 and Fabric 3, printed with printing pastes based on reactive dyestuff C.I. Reactive Blue 19, C.I. 61200.

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Flame retardant and surface properties of designed aramid fabrics

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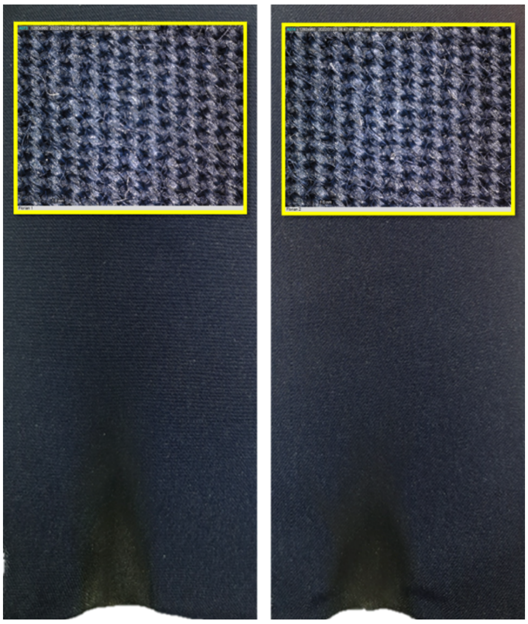
Abstract:
Flame retardant (FR) textiles represent one of the specific and significant niche on the world textiles market, designed to protect against fize hazards. Most textile materials are flammable, so it is necessary to make them less flammable. Inherent FR fabrics are designed from fibres when there is no need to carry out additional treatments to achieve the desired FR effects.

The proposed concept covers a production and implementation of the inherent FR fabric designed in twill from aramid fibres. The first one refers to the finishing stage in the production of yarn, where two fixation media are varied by selection of paraffin and a steam for the fixation of protruding fibres in yarn (Figure 1). The second refers to durability of designed fabric through exposure to processes of washing and artificial ageing. Functional and surface properties of designed FR fabrics will be examined before and after washing and ageing. Laboratory evaluation of fire performace will the done by vertical burning test, LOI (Limiting oxygen index) and micro cone calorimetric (MCC) evaluation criteria: total heat release (THR), heat realase rate (HRR) and the peak of heat realase rate (pkHRR). Surface characterization of samples before and after washing and ageing will be examined by scanning electron microscopy (SEM). Other properties, such as color change and pH of an aqueous extract will contribute to the appearance and assessment of the risk from migrating particles.

Keywords: textiles, flame retardancy, aramid, Kermel®, paraffin, steam, wash durability, persistence in ageing, surface examination, SEM, flame retardancy, LOI, MCC, color.



a) **b)**

Figure 1: Figure a illustrate the digital image of FR fabric weaved in twill from the yarn finished with paraffin; Figure b illustrate the digital image of FR fabric weaved in twill from the yarn finished with a steam.

The question is how the selected fixation media in a production phase and ageing/washing processes in the implementation phase affect on FR properties and surface of designed inherent fabrics.

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Surface properties of polyester fabrics

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Abstract:

Large amounts of plastics used for a different purposes caused a certain environmental problems. More or less, regular or irregular, micro or nano sized particels end up in the marine environment and pose a major risk to organisms living there. Analysis of microplastic samples (MP) from the environment, shown that textile fibres are common source of pollution. However, according to the data since 2019, approx. 35% belong to textile fibres, where is polyester (PES) a dominant source of contamination.

Facts from a global perspective, have shown that the washing process is one of the major sources of released MP particles into effluents. Structural properties of the textile material are important for assessment of lifetime.

This study will be focused on the characterization of polyester fabric after exposure to artificial ageing and washing cycles (Figure 1). Objective evaluation of pristine and treated samples of polyester fabrics will be examined by three methods. Fabric Touch Tester (FTT) will be used for characterization the physical properties on both surface side, top and bottom side, assessing total comfort (smoothness, softness, and warmth). The objective evaluation of fabric quality and performance will be performed through the measurement of the following properties: thickness, compression, bending/stiffness, surface roughness, surface friction and thermal properties.

An additional assessment of the surface properties of untreated and treated polyester fabrics will be done by zeta potential. On the basis of the characterisation parameters, a multi-variant analysis (MVA) will be carried out with a view to establish the similarities and differences between individual polyester fabric samples before and after these treatments.

Keywords: textiles, polyester, washing, artificial ageing, total comfort, zeta potential, multivariate analysis.

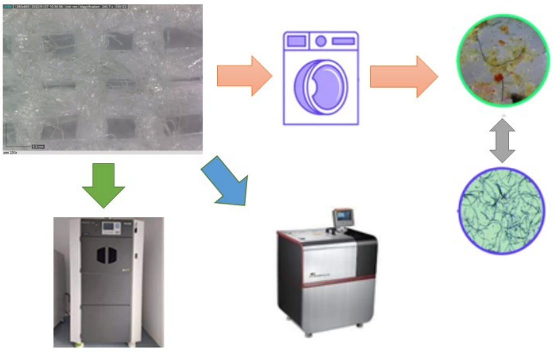

Figure 1: Figure illustrates the digital image of polyester fabric weaved in canvas that will be subjected to artificial ageing and washing

The study addresses two questions:

- how an exposure to artificial light and wash media will impact on the surface properties of polyester fabric
- applicability of MVA for surface evaluation through selected parameters.

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Benefits of low-temperature aging of superelastic NiTi alloy

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Abstract:

Precipitation in superelastic Ni-rich NiTi alloy affects material properties such as fatigue life, tensile strength, or thermos-mechanical response. In this work, a nonconventional method of pulse heating by the electric current was employed to recover cold-worked NiTi wires and set the initial microstructure without precipitation. Thus, the impact of recrystallization processes, and aging on mechanical properties can be separated. After the initial pulse heating, the NiTi wires were subjected to various aging treatments at 200 °C – 400 °C for 1 h – 5 h. The aging at an appropriate temperature allows a fluent and predictable adjustment of superelastic response with increased tensile strength. However, the aging of samples with an increased gain size (d>250 nm) yields lower improvement in tensile strength and stability of cyclic superelastic response as the larger grain size offers a lower number of nucleation sites.

Moreover, TEM analysis was performed to determine the mean size and distribution of Ni-rich precipitates in the NiTi matrix. Precipitation occurs predominantly on grain boundaries during aging at 400 °C, and functional stability in cyclic loading remains insufficient. Thus, aging at low temperatures (T ~ 300 °C) was employed, which yields approx. 5nm precipitates and substantially improves the homogeneity of precipitates distribution improving the stability of superelastic response and increasing tensile strength (Fig.1). Low-temperature aging is beneficial, especially in microstructures with large grain sizes, as these would be otherwise severely unstable in a cyclic thermo-mechanical loading.

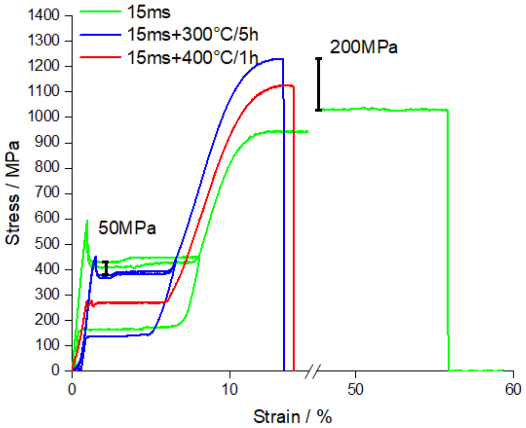

Figure 1 Figure illustrating effect of heat-treatment on stress-strain response of NiTi wire at 20 °C. Response of wire subjected to: pulse-heating for 15 milliseconds (Green), pulse-heating for 15 ms followed by annealing 400°C/1h (Red), and pulse-heating for 15 ms followed by annealing 300°C/5h (blue).

Keywords: NiTi, aging, superelasticity, functional fatigue

Surface degradation study of historical crown glasses from 15th – 17th century

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Abstract:

Crown glasses were commonly used in the late Middle Ages and the early Modern Age as a form of glazing characteristic for secular and sacred buildings [1, 2]. In this work, the set of historical crown glass samples was studied especially in terms of surface degradation caused by interaction with the surrounding environment. Analyzed glasses were found to be in relatively good condition, however, some iridescence, partial surface exfoliation, and pitting corrosion appeared. (Figure 1). The following research methods were used to assess the degree of corrosion and its products on the surface: Scanning Electron Microscopy (SEM) including Energy Dispersive Spectroscopy (EDS), Optical Microscopy (OM), Atomic force microscopy (AFM) and Raman spectroscopy. The obtained results indicate a significant influence of environmental parameters and glass composition on susceptibility to corrosion.

Keywords: historical glass, corrosion, crown glass, Raman spectroscopy, optical microscopy, AFM, SEM, archeometry.

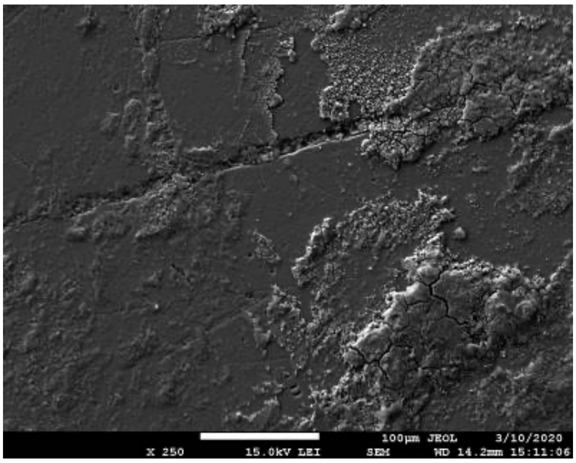

Figure 1: SEM images of the crown glasss surface with visible corrosion.

References:

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Acknowledgments:

This work was supported by The Slovak Grant Agency for Science under grant No VEGA 2/0091/20, VEGA 1/0155/22 and by the Slovak Research and Development Agency project APVV SK-PL-18-0062, and the project Centre for Functional and Surface Functionalized Glass (CEGLASS), ITMS code is 313011R453, operational program Research and innovation, cofunded from European Regional Development Fund.

Thermomechanical properties of silicate and phosphate glasses

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Abstract:

Knowledge of the interdependence between structural and thermal and thermomechanical properties of oxide glasses contributes to expanding their practical use. Thermophysical methods are intensively used in science and technology [1-3]. However, we recognize different levels of their application. Regular measurements of selected properties of glass and glass melts are performed on commonly produced glass as part of inspections or changes in production technology. Of course, in many cases this is related to changes in the raw materials used, or refractory materials or logs. In this case, it is necessary to pay attention to the measurements of viscosity, glass transition temperature and linear coefficient of thermal expansion of glass. The studied glasses were prepared from analytically pure raw materials - oxides and carbonates, melted in a platinum - rhodium crucible. The homogeneity of the glasses was ensured by manual mixing during melting. After melting and pouring onto a metal plate, the glasses were tempered in a muffle furnace and then cooled to room temperature. The chemical composition of the prepared glasses was determined by X-ray fluorescence analysis (BRUKER, Tiger S8) and inductively coupled plasma atomic emission spectroscopy (ICP OES, VARIAN Vista 240 FS). Thermal behavior was monitored by DSC at 5-20 °C/min and by TMA at 5 °C/min. and a pressure of 5mN. From the data obtained from the DSC and TMA curves, it was possible to use the Rough Criterion [4] in the form $K_{gl} = (T_c-T_g) / (T_m-T_c)$ to observe the tendency of glass formation, while a higher K_{gl} value means higher thermal stability and tendency to glass formation. The measured temperature dependences of the low-temperature viscosity using the TMA instrument by the method of axial defothing of the chips were in all cases very well approximated by the Andrade viscosity equation. The standard deviations of the approximation were in all cases at the level of the experimental error of viscosity determination.

Keywords: silicate glass, phosphate glass, thermal expansion, viscosity, activation energy

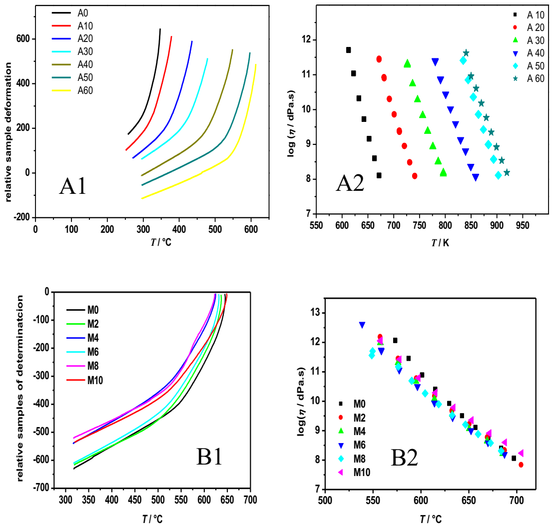

Figure 1: Thermodilatometric cooling curves of phosphate (A1) and silicate (B1) glasses. Dependence of viscosity logarithm on reciprocal thermodynamic temperature for phosphate (A2) and silicate (B2) glasses.

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Acknowledgments

This study was supported by the Slovak Grant Agency for Science under the grants and VEGA 2/0091/20 and VEGA 1/0152/22 and the project Centre for Functional and Surface Functionalized Glass (CEGLASS), ITMS code is 313011R453, operational program Research and innovation, co-funded from European Regional Development Fund.

The surface layer study of binary glasses.

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Abstract:
A set of binary alkali silicate glasses with different contents of Na_2O and K_2O was melted. The composition of the prepared glasses was determined by Xray fluorescence elemental analysis (XRF). Glass samples were exposed to the corrosion environment of 36% hydrochloric acid and the exposure time was recorded. A wide range of exposure times was chosen in order to cover both the initial stage of corrosion process and the growth of larger corrosion products [1-3]. Glass samples were measured by scanning electron microscopy (Fig. 1) and Raman spectroscopy (Fig. 2). The spectra were compared with Raman spectra of original pristine glasses in order to observe structural changes induced by corrosion within the surface layer. The usage of confocal Raman spectroscope enabled the measurement of Raman spectra from the depths of few micrometres to document the range of structural changes. The results suggest the depolymerisation of silicate structure due to the growth of the corrosion layer on the surface. The decrease of D2 peak points at the decomposition of three-membered rings. In addition, it is assumed that the Si-O-Si angle changes within the surface layer.

Keywords: glass surface; glass structure, sodium silicate glass, potassium silicate glass, Raman spectroscopy, glass corrosion.

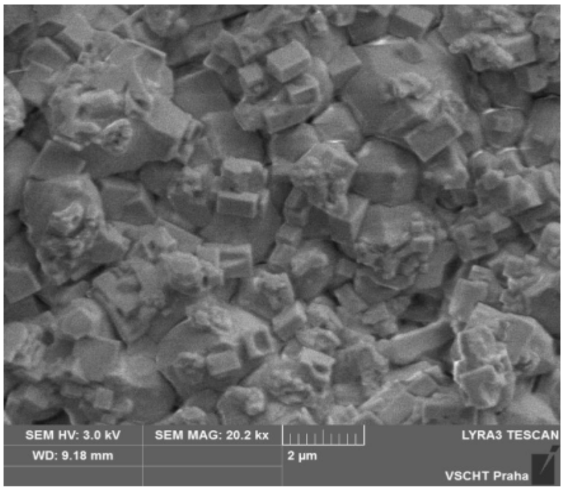

Figure 1: SEM image of the surface of 3Na sample.

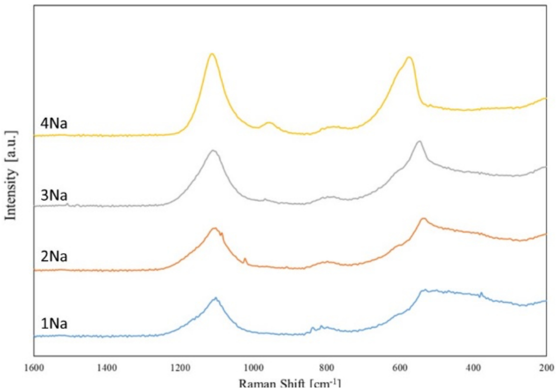

Figure 2: Raman spectra of four binary sodium silicate glasses with increasing amount of sodium.

References:

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Acknowledgment:
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Zn-rich coatings dried with infrared (IR) radiation

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Abstract:
Zinc-rich primers (ZRP) have unique property of metal protection even when there is a slight mechanical damage to the coating due to its cathodic protection mechanism. They are often used as primer coatings in various aggressive environments such as offshore, industrial, etc [1]. For the successful protection, the Zn-rich coatings need to be applied to clean surface, properly mixed and dried. There is an increasing tendency to find more efficient drying methods while maintaining the good coating protective properties due to the technical and economic factors [2]. Infrared (IR) drying technology presents itself as one such method. The aim of this paper is to determine the influence of different IR drying parameters on Zn-rich coating protective efficiency and the drying speed. The observed parameters are the distance of the samples from the IR radiation source and the thickness of the mild steel plates. Pull-off test was done on the samples after drying to determine if the coatings were chemically cross-linked and ready for exploitation. Coating resistance was determined electrochemical impedance spectroscopy (EIS) and corrosion properties were evaluated with accelerated corrosion tests. The results show increase in the drying time with the increase in the distance from the IR radiation source as well as the thickness of the samples. However, when comparing conventional drying methods and IR technologies, IR drying achieves significant savings in drying times with no negative effect on coating protective properties.

Keywords: zinc-rich primers, infrared drying, electrochemical impedance spectroscopy, corrosion

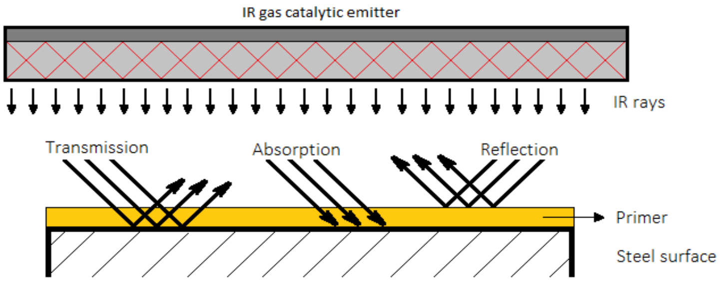

Figure 1: IR curing process of primer layer

References:

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Bioactive spray based on green synthesis silver nanoparticles

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Abstract:

Due to the current epidemic of the coronavirus (COVID-19), the main cause of the epidemic is bacteria and viruses spreading. Therefore, bioactive spray containing silver nanoparticles (AgNPs) were studied and developed in this study (Figure 1). The synthesized AgNPs could be achieved from an environmentally friendly process with use of extract spent coffee grounds (ex-SCG) as a biological reducing agent combined with citric acid. Different silver nitrate concentrations of 50, 100 and 150 mM were used to produce AgNPs-50, AgNPs-100, AgNPs-150, respectively. Based on the obtained results AgNPs-100 showed the best distribution of silver nanoparticles. The coated fabric with AgNPs via spraying had the highest self cleaning ability of 12.61%. In addition, the AgNPs-100 spray could inhibit the growth of bacteria up to 99.99% for *Escherichia coli* (*E. coli*) and 99.99% *for Staphylococcus aureus* (*S. aureus*). The antiviral activity was observed within 1 minute for coated fabric with AgNPs-100. Hence, the obtained AgNPs-100 spray could have a potential to use as sanitizer spray for reduction of inflection risk from virus and bacteria.

Keywords: spray coating, silver nanoparticle, extract spent coffee grounds, citric acid, self cleaning, reduction of inflection risk, antiviral, antibacterial, biomedical applications.

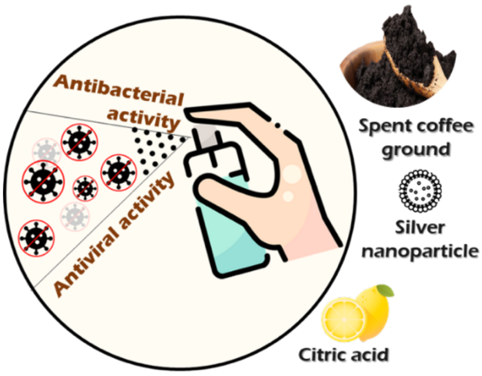

Figure 1: The figure depicted the concept of spray coating on the parameters affecting the green synthesis and biological activity.

References:

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Aspergillus for nanoparticle: Possibilities and challenges of biomediated nanoparticle synthesis of silver nanoparticles

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Abstract:

Nanoparticle commodities are of ever increasing importance, with precious metal nanoparticles especially, being increasingly integrated into new materials and consumer products. (Stavis, 2018) Green chemistry synthesis routes for nanoparticles, including microbial synthesis schemes, are therefore of increasing interest, as they can alleviate high energy costs or usage of harmful chemicals in conventional, physicochemical synthesis routes. Various microorganisms are capable of building metallic nanoparticles intra- and extracellularly and especially fungi are known to give high yields. (Narayanan, 2010) Fungi of the *Aspergillus* species in particular are promising candidates for nanoparticle synthesis, as they show exceptional protein and secondary metabolite excretion rates. (Meyer, 2010) Here, the extracellular synthesis of silver nanoparticles by three different *Aspergillus* species is investigated and compared. Extracellular reduction of diluted silver solutions yielded protein-coated nanoparticles of different sizes and dispersities, depending on the *Aspergillus* species used. High yields can be achieved from diluted solutions. Formation kinetics and colloidal stability was found to be species-dependant and linked to lighting conditions during synthesis. Colloidal stability of the yielded nanoparticle fractions was identified as challenge, as product quality is lost due to agglomeration, which was successfully subdued by controlling pH during synthesis. Biomediated synthesis by *Aspergillus* species pose a cost-effective, environmentally-friendly way of generating silver nanoparticles, that is especially interesting for valorizing dilute waste solutions from industries such as the pharmaceutical und galvanic application fields.

Keywords: silver nanoparticles, green synthesis, Aspergillus, waste valorisation.

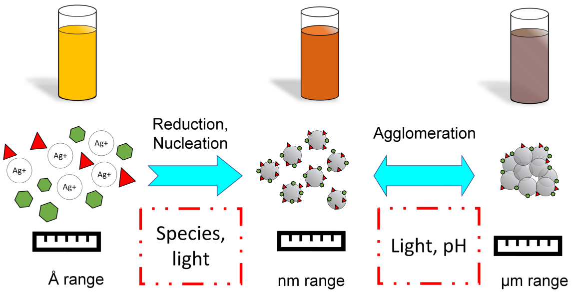

Figure 1: Reduction of silver nanoparticles by means of Aspergillus species: Insights into parametrs affecting formation and colloidal stability

References:

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Peptide Targeted Gold Nanoplatform Carrying miR-145 Induce Antitumoral Effects in Ovarian Cancer Cells

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Abstract:

One of the recent attractive therapeutic approaches for cancer treatment is restoring downregulated microRNAs. They play an essential muti-regulatory role in cellular processes, such as proliferation, differentiation, survival, apoptosis, cell cycle, angiogenesis, and metastasis, among others. In this study, a gold nanoplatform (GNPF) carrying miR-145, a downregulated microRNA in many cancer types, including epithelial ovarian cancer, were designed and synthesized. For targeting purposes, the GNPF was functionalized with the FSH33 peptide, which provide selectivity for ovarian cancer, and loaded with the miR-145 to obtain the nanosystem GNPF-miR-145. The GNPF-mir-145 selectively was incorporated in the A2780 and SKOV3 cells and significantly inhibited cell viability, migration, and exhibited proliferative and anchorindependent growth capacities. Moreover, it diminished VEGF release and reduced the spheroids size of ovarian cancer through the damage of cell membranes, thus decreasing cell viability, and possibly activating apoptosis. Thereby, the feasibility of the GNPF structuration and the simplicity of the miR conjugation make it a platform with potential multi-possibilities of cargo incorporation. Thus, one or multiple short double-strand RNA molecules or mixtures of them, raising the possibility to create powerful tools to achieve a better biological response. These results provide important advances in developing miR-based therapies using nanoparticles as selective vectors and provide the approaches for the *in vivo* evaluation.

Keywords: Ovarian Cancer; Nanoplatform; microRNA

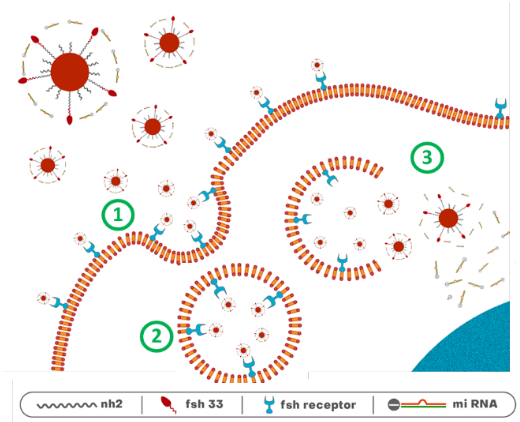

Figure 1: Schematic representation of the gold nanoplatform carrying miRNA and its process of recognition (1) for target cells, endocytosis (2) and delibery of miRNAs (3) into the cytoplasm to generate the cellular effects.

Funding: This work was supported by Fondecyt 3190547, Fondecyt 1160139, Fondecyt 1190623, Fondecyt 1211482, PAI 77200057, and Fondap 15130011.

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Brain Drug Delivery of Riluzole by means of Lactoferrin Functionalized Nanostructured Lipid Carriers

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Abstract:

Amyotrophic lateral sclerosis (ALS) is a neurodegenerative disease with a fatal outcome. It is characterized by progressive degeneration of motor neurons, having a median survival of 2 to 5 years [1]. The existence of the blood-brain barrier (BBB), severely restricts the access to the brain of therapeutics used in the treatment of ALS, including riluzole. In this sense, lipid nanoparticles (NPs), especially when conjugated with surface ligands, can enhance drug delivery and improve targeting efficiency across the BBB [2]. We report the formulation and characterization of functionalized nanostructured lipid carriers (NLC), to increase riluzole brain delivery due to the synergic effect with the ligand lactoferrin (Figure 1) [3]. The NPs were prepared by the sonication technique. Lactoferrin conjugation was achieved via carbodiimide chemistry. The NLC were characterized with respect to their physicochemical properties (size, zeta potential, polydispersity index) as well as their stability, encapsulation efficiency, morphology, in vitro release profile, and biocompatibility. Furthermore, crystallinity and melting behavior were assessed by DSC and PXRD, and lactoferrin coupling by FTIR and protein quantification studies [3].

The NPs remained stable over at least 3 months, exhibiting initial mean diameters between 180 and 220 nm, a polydispersity index below 0.3 and high encapsulation efficiencies (between 94-98%). TEM images confirmed the size obtained by DLS, showing also that NLC were almost spheric in shape, with a smooth surface. FTIR spectra corroborated the formation of the amide linkage and protein quantification using the Bradford assay revealed a high coupling efficiency (97%), which also supports the successful lactoferrin functionalization of the NPs [3].

In an MTT assay, the NPs did not cause a substantial reduction in the viability of NSC-34 and hCMEC/D3 cells at a riluzole concentration up to 10 µM, being therefore biocompatible (Figure 1). These results suggest that the functionalized NLC are a suitable and promising delivery system to target riluzole to the brain [3].

Keywords: blood-brain barrier (BBB), amyotrophic lateral sclerosis (ALS), lipid nanoparticles, nanostructured lipid carriers (NLC), riluzole, lactoferrin, functionalization, brain drug delivery.

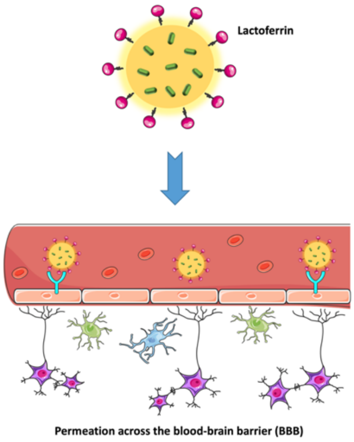

Figure 1: Figure illustrating the permeation of lactoferrin functionalized NLC loaded with riluzole across the BBB.

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Innovative biogels delivering miRNAs into skin models. Wound healing applications within the EuroNanoMed project TENTACLES

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Abstract:
An ideal wound dressing material should be biocompatible, able to protect the wound from bacterial infections, prevent excessive fluid loss and maintain a moist healing environment [1]. To date, many polymeric materials have been clinically used for wound dressing [2], but, actually, none of them contains multiple 'active' therapeutic molecules at the same time. Nanogels are polymeric drug delivery systems made by one or more molecules linked together by physical and chemical linkages to form hydrogels [3]. Nanogels, referred also as hydrogel nanoparticles, have the characteristics of both hydrogels and nanoparticles (NPs) [4]. Nanogel drug delivery systems are able to protect effectively active substances from oxidation and degradation [5], therefore macromolecular drugs and therapeutic agents such as siRNA [6-8], DNA [9] and oligonucleotides [10,11] can be stably loaded into these systems. On this purpose, we preliminary prepared and characterized several commercial (Pluronic-F127 and Ca^{2+}-crosslinked alginate), and synthetic biogels (Gelatin-, chitosan- and chondroitin sulphate-methacrylates) containing iron nanoparticles and miRNAs. We analyzed the differences of these biogels and demonstrated their ability to retain the iron oxide nanoparticles within their bulk structure and release miRNAs at the same time. Preliminary results showed the great ability of alginate to entrap both iron oxide nanoparticles and microRNA, and the efficiency of GelMA and pluronic biogels to differently release microRNAs and NPs. Moreover, these hydrogels are also able to heat by electromagnetic irradiation, owing to the presence of iron oxide NPs. These biogels have therefore multifunctional properties and by modulating each of these properties is it possible to create even more complex systems.

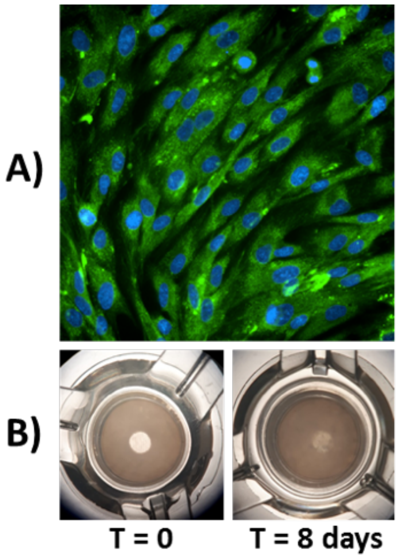

Figure 1: A) miRNA release into HFF-1 fibroblasts and B) healing of a skin wound after one week.

In this contribution, we will illustrate the potential application of these biogels, their physicochemical properties and toxicity profiles on skin models (cells and organoids), and the delivery of selected miRNAs for the modulation of important patways related to skin regeneration.

Keywords: Nanogel, Wound healing, miRNAs, Heat shock proteins, Nanoparticles, Thermal treatment

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Design Optimization of Memantine Loaded Micro/Nanomotor for Alzheimer's Disease

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Abstract:

One of the most exciting steps in nanotechnology is certainly phenomenon of gaining mobility to the synthesized materials. Synthetic micro/nanomotors (MNMs) are one of the newest nanotechnology systems that have been introduced within the last decade. Synthetic MNMs designed for this purpose are molecular or nanoscale structures that have the ability to convert energy into motion. MNMs and their movement ability (due to their propulsion mechanisms) allow access throughout the whole human body, leading to, localized diagnosis and treatment with increased precision and efficiency.Synthetic MNMs are classified into 2 groups according to their propulsion characteristics: i-Catalytically-Powered MNMs and ii-Physically Powered MNMs. The movement mechanism in Physically Powered MNMs can be provided with Magnetic field, Acoustic field, Electrical field, Ultrasound, and Light effects. Studies indicate that MNMs which are activated and moved under a magnetic field can offer advantages in terms of real-life applications.

Alzheimer's Disease (AD) is one of the most frequently occurring diseases, especially in those over 60 years. It is a neurodegenerative disease of the central nervous system and is classified under dementia. The major boundary for the treatment of AD is the Blood Brain Barrier. Tight junctions of the BBB, limit the passage of active pharmaceutical ingredients from systemic circulation to the brain. Nanotechnology brings new insights for access to the BBB with localized and active drug delivery. For this purpose, we have introduced Memantine Loaded MNMs for the first time. The nanomotors were prepared electrochemically according to the membrane-die technique. One side of the cylindrical alumina membranes (200 nm) has been made conductive by being coated with a thin strip of silver (Ag) by sputtering method in order to serve as a working electrode.Then, these coated membranes were placed in the teflon electrochemical cell. In the teflon cell, Pt wire was used as the counter electrode and Ag/AgCl electrode was used as the reference electrode. Based on the amino acid monomer, poly-L-lysine was deposited on the surface. After that, deposition studies of gold (Au) and nickel (Ni) metals were carried out. The controlled movement properties of the motors were optimized under microscope. Finally, Memantine interaction studies were carried out by incubating Memantine with the synthesized nanomotors at different times and %26,3 incubation were successfully obtained.

Keywords: micro/nanomotors, Alzheimer's disease, memantine, magnetic propulsion

Figure 1: Optical microscopic image of the wire (rod) motors based on polymeric layer.

Acknowledgement: This study was kindly supported by TÜBİTAK project with the number 219S811.

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Protein aggregation mechanisms: human H-ferritin self-assembly for costructions of new nanomaterials

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Abstract:
In nature, many proteins can self-assemble forming supramolecular complexes. These structures can be characterized by one-dimensional organization as in the case of fibrillar systems, two-dimensional such as films or functionalized surfaces, and three-dimensional as in the case of hydrogels and nanocages.[1] Among nanocage systems, ferritin (Ft) occupies a special position. Indeed, Fts of different origins share common, interesting features, such as a hollow-spherical structure, high thermal and chemical stability, and high solubility.An interesting feature of Ft nanocages is their capability to disassemble and reassemble at extreme pH which, together with the hollow structure and the easy production protocols, makes them suitable nanosystems for molecules encapsulation. Furthermore, ferritin surface can be chemically or genetically functionalized for targeting toward specific cells. Within this interesting family, Human Ft (hFt) seems particularly interesting for its low immunogenicity. hFt is made up of 24 subunits that naturally self-assemble to form a nanocage structure. The cage has octahedral symmetry, an external diameter of 12 nm and an internal one of 8 nm. Two types of subunits can be distinguished: L chains, light, and H chains, heavy.[2] H chains have a high affinity for the TfR1 transferrin receptor, over-expressed on the cell surface of different cancer cell lines.[3] For these reasons, we focused on nanocages constituted by the human H-chain (hHFt) for possible use as cargos for transport and delivery of different drugs. We analyzed in detail the disassembly/reassembly mechanism under different physico-chemical conditions, by using a multimethodological biophysical approach. The explored protocols allowed us to study the encapsulation in the nanocage and the release of molecules of different nature, including metallodrugs, polypeptides and bioactive compounds. First experiments revealed that at acidic pH the Ft nanocage is disassembled, whereas at alkaline pH the the nanocage is still present (Figure 1). The quaternary structure can be recovered upon restoring the pH at physiological values, even if a small amount of protein is lost in the process and the homogeneity of the supramolecular structure upon reassembly is still unclear. Furthermore, very often the molecules to be encapsulated are not stable under the extreme pH conditions necessary to dissociate the hHFt nanocages. Thus, we expand the study to analyze alternative agents to drive the disassembling/assembling process of hHFT nanocages. Here, we report a comparison of the different protocols explored and the characterization of the structural and functional properties of different nanosystems.

Keywords: protein assembly, nanosystems, ferritin nanocage, extreme pHs, encapsulation, protein-loaded ferritins.

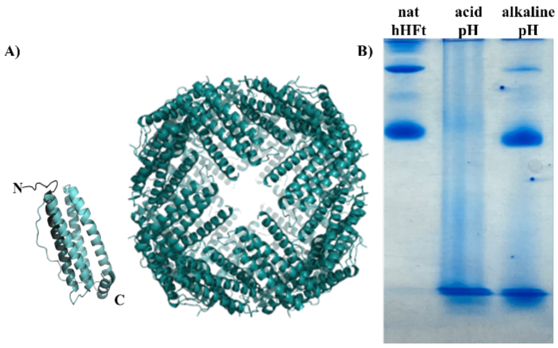

Figure 1: A) Cartoon representation of ferritin subunits and cage structure (PDBcode: 5N27); B) native PAGE of hHFt at physiological, acid and alkaline pH.

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Targeting Iron Metabolism in Cancer to Induce Ferroptosis: A Type of Programmed Cell Death

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Abstract:
Tumour cells display metabolic flexibility in order to maintain rapid proliferation and enable metastasis to other organs. Alterations in tumour cell iron metabolism, established by increasing the expression of the transferrin receptor protein 1 (TFR1), correlates with poor prognoses in cancer[1]. However, increased cellular iron can participate in the generation of potentially deleterious free radicals, driven by the Fenton reaction. Free radicals are then readily available to attack lipid membranes; producing toxic lipid peroxides and subsequently induce ferroptosis; an iron-dependent cell death pathway[3] (Figure 1).

Cancer cells are able to evade ferroptotic induction through the over-expression of glutathione peroxidase IV (GPX4), which uses glutathione to catalyse the conversion of lipid peroxides into their equivalent alcohols (Figure 1).

Recent studies have shown that therapy-resistant cancers are vulnerable to the induction of ferroptosis. However, current ferroptotic activators are unable to circulate throughout the body, therefore alternatives are required. Iron oxide nanoparticles can be cytotoxic to human cancer cells and therefore could be exploited for cancer therapy[2]. Results so far indicate that polyethylene glycol, PEGylated iron oxide nanoparticles alone have little effect on inducing ferroptosis in cancer cells. However, coating iron oxide nanoparticles with a ferroptosis incuding-agent has shown promising results in reducing viability in a panel of cancer cell lines.

We hypothesise that targeting therapy-resistant cancer cells with iron oxide nanoparticles will induce ferroptotic cancer cell death.

Keywords: Cancer, iron metabolism, transferrin receptor protein 1, Fenton reaction, free radicals, lipid peroxides, ferroptosis, iron oxide nanoparticles, PEGylated, glutathione peroxidase IV, therapy-resistance.

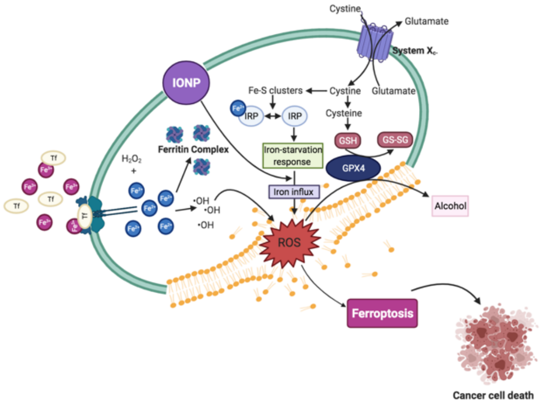

Figure 1: Figure illustrating the biological relationship between the Fenton reaction and ferroptosis, via the production of free radicals to the reduction of lipid peroxides to their equivalent alcohols. Iron oxide nanoparticles (IONP) also induce ferroptotic cancer cell death.

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Antibacterial chitosan-graphene nanocomposites

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Abstract:

One of the major trends of research in bio-based polymer industry involves their manufacturing as bioplastics for food packaging and medical products including antimicrobial agents. Nanocomposites made of a polysaccharide such chitosan could be excellent functional films. Chitosan is a biocompatible, fully-degrable, non-toxic biopolymer, that easily undergoes chemical and enzymatic modifications, which allows obtaining derivatives with increased biological activity. These features account for implementing chitosan scaffolds in various fields including scavenging chemicals, tissue-engineering, wound-dressing, drug-release and food-packaging. In particular the excellent film-formingability of chitosan opened great opportunities for bio-based wound-dressing materials. However, its poor mechanical strength constitutes a serious impediment for this specific application. The addition of a low amount of nanosized fillers derivatives provides a way to improve its mechanical properties as well as antimicrobial activity. A rising interest in graphene and its derivatives has rcently been noted. The aim of this study was investigating the antibacterial potential of chitosan-reinforced-graphene-films against the reference strains of gram-positive and gram-negative bacteria. Moreover, the mechanism of antibacterial action of tested nanocomposites was evaluated using scanning electron microscopy and confocal microscopy analysis.

The obtained results showed that chitosan reinforced graphene nanocomposites possesses strong antibacterial properties against tested Gram positive and Gram negative strains, especially towards *Staphylococcus aureus* and *Staphylococcus epidermidis* strains (90% growth inhibition). Moreover, the bacterial cell membrane was recognized as one of the possible targets of the antibacterial action of the chitosan-reinforced-graphene-films.

Because of the growing interest in bio-based polymers, bio-nanocomposites will play a pivotal role in the nearest future. Graphene incorporation in chitosan films allows potential antibacterial activities, compared to native chitosan films.Acknowledgement.

The study was founded by the National Science Centre, Poland, no. 2017/25/B/NZ9/02900.

Keywords: chitosan nanocomposites, graphene, antibacterial activity, biomedical applications.

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Synthesis of PLGA, PCL and its Nano-Fabrication for the Tissue Engineering Application by using Electrospinning and Melt Pining Technique

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Abstract

Polylactic glycolic acid PLGAand PCL is most important polymer in biomedical applications the degradation of kinetics modified by co-polymerization ratio of monomer. In this interest Biodegradable and biocompatible polymers are use in controlled drug delivery systems, in the form of implants devices for skin bone, and dental repairs, Microwave irradiation on as a heating source for polymerization reactions is a rapidly growing branch in polymer science current research shows both the microwave and heating synthesis is efficient alternative which takes less time for polymerization. With microwave synthesis polycondensation, free and controlled radical polymerization, and ring opening polymerization (ROP) can be done. The characterization of Polycaprolactone was done by Fourier Transform Infrared Spectrophotometer (FT-IR), scanning electron microscopy (SEM), The polymer interactions were checked by Differential scanning calorimetric (DSC) and the XRD analysis was carried out to determine structural changes PLA/PCL nanofabrication done by electrospinning Technique for biomedical applications. PLGA synthesis done by convectional method, with study of various parameter such as time, temperature, monomer and catalyst ration. Input monomers and the reaction products are analyzed here. Important characteristics, melting temperature, glass transition temperature, thermal stability, chemical composition and the ratio of the monomers in the synthesized and copolymer, were obtained from these analyses. These results helped to infer the absence of residual monomers in the synthesized copolymersPCL done by microwave assisted method.. The PLGA micro particles are one of the most successful new drug delivery systems (DDS) in labs and clinics. Because of good biocompatibility and biodegradability, they can be used in various areas, such as long-term release systems and the tissue engineering.

Keywords: Biocompatible, Biodegradable, Electrospinning, Melt spinning, Polymerization, Synthesis, PLGA PCL, Nanofabrication.

Recycling of used face mask to white light emitting carbon dots

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Abstract:

Covid-19 pandemic has escalated the use of surgical mask and N95 mask across the globe that takes hundreds of years to degrade and finally end up as micro plastics in soil. In this work we report recycling of used surgical mask, N95 mask into white light emitting carbon dots (CDs). Further the fabricated CDs are characterized using UV-absorption emission spectroscopies. Using our unique recycling technique, broadband single system white light emitting CDs with broad absorption and emission bandwidth of ~ 143 nm and ~124 nm are fabricated using used surgical mask and N95 mask respectively. This work will address the issue of plastic waste pollution and these dots find applications as active emitters in artificial lighting devices.

Keywords: face mask, N95. Surgical mask, white light, carbon dots

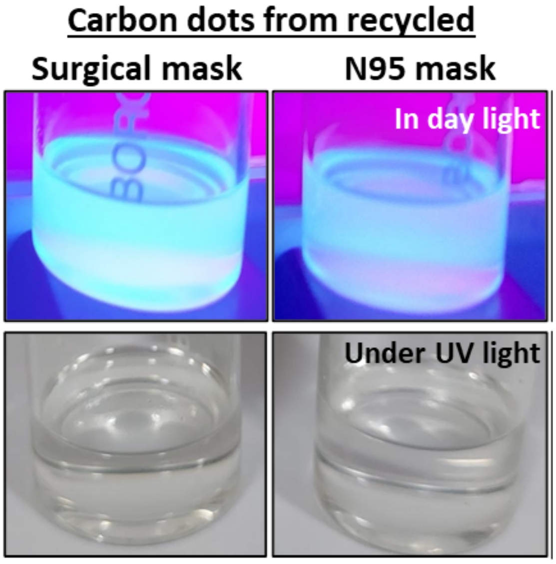

Figure 1: Figure showing white light emitting carbon dots from recycled surgical and N95 mask. These dots emit white light under UV illumination.

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Rapid, accurate detection of COVID-19 utilizing novel isothermal nucleic acid amplification

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Abstract:
The novel respiratory infection coronavirus disease (COVID-19) caused by Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2), which occurred in December 2019, has developed into a pandemic. Herein we describe a COVID-19 detection method based on the Nicking and Extension chain reaction System-Based Amplification (NESBA) by utilizing multiple gene detection of SARS-CoV-2. The NESBA primer set was simply designed to contain the T7 promoter sequence and nicking site at the 5' end of target binding region complementary to the E and N genes of SARS-CoV-2. Exponential amplification of RNA amplicons due to repeated nicking and extension chain reaction contributes to high sensitive detection and rapid detection time (< 30 min) with E and N genes down to 10 copies per reaction volume, respectively. We also validated clinical applicability of our method using 98 clinical samples collected from suspected COVID-19 patients, determining 30 positive and 68 negative samples with 100% sensitivity (95 % CI 88.43 % to 100.00 %) and 100% specificity (95 % CI 94.72 % to 100 %) for both E and N genes. Therefore, this strategy could be a great application value in the on-site clinical diagnosis of COVID-19 and would serve as a promising platform to achieve point-of-care (POC) molecular diagnostics for early diagnosis of various infectious diseases.

Keywords: COVID-19, SARS-CoV-2, RT-PCR, isothermal nucleic acid amplification, NESBA, clinical diagnosis, POCT.

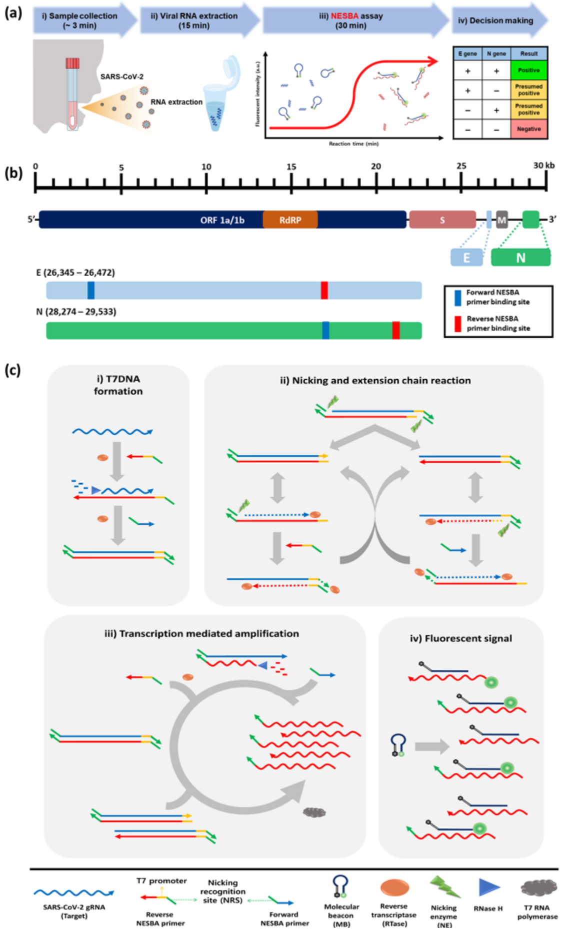

Figure 1: The overall procedure of the COVID-19 diagnosis by NESBA. (a) The workflow of the COVID-19 diagnosis. (b) The SARS-CoV-2 genome map (GenBank accession number: MN908947) and target regions of the NEBSA. (c) Schematic illustration of the NESBA for target RNA detection. The arrow indicates the 3' end of the nucleic acid strand.

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Multiplex reverse transcription loop-mediated isothermal amplification combined with nanoparticle-based lateral flow biosensor for the diagnosis of COVID-19, *Biosens. Bioelectron.*, 166, 112437-112443.

Titanium Coating on Laser Roughened PEEK for Spinal Implant

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Abstract:

Current spinal interbody fusion cages are most widely adopted from polyetheretherketone (PEEK) due to its favorable biomechanical properties and X-ray radiolucency characteristics. Unfortunately, the smooth and bioinert surface of PEEK may limit the osseointegration and inhibit bone fusion. Plasma spraying, providing porous and rough titanium layer over the PEEK spinal implant, has been commercialized in clinical application though, this study aims to develop an alternative approach by first laser roughening PEEK surface, followed by high power impulse magnetron sputtering (HIPIMS) to deposit a strongly adhered titanium layer for improving osteointegration of PEEK spinal implant (Figure 1). The experimental results showed that properly controlled laser condition gives micrometer-scale topography over the PEEK surface as opposed to the smooth bare PEEK. After HIPIMS deposition, the obtained titanium film presented an adhesion of 5B grade even after immersion in simulated body fluid (SBF) environment for 28 days based on the Scotch-tape adhesion test. Such excellent film adhesion performance is ascribed to the advantage of high ion energy and high-density plasma characteristics of the HIPIMS discharge. In addition, the titanium film on roughened PEEK presented better osteoblast compatibility and osseointegration than the commercial product, so as to provide high spine stability after implantation. Finally, the long-term assessment results revealed the high stability and no degradation concern for the modified PEEK, which can avoid the malignant reaction between implant and host to ensure the safety after implantation in the human body. In summary, the two-step surface modification on PEEK satisfies the requirements for enhancing osseointegration, suggesting clinical application consideration.

Keywords: polyetheretherketone (PEEK) cage, laser roughening, high power impulse magnetron sputtering (HIPIMS), titanium film.

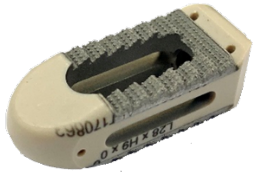

Figure 1: Ti coating on laser roughed PEEK cage.

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Lipase-catalyzed acylation of bio-oil enriched with levoglucosan: antibacterial and biosurfactant studies

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Abstract:
Studies involving the transformation of lignocellulosic biomass into high value-added chemical products have been intensively conducted in recent years. Levoglucosan (1,6-anhydroglucopyranose (LG)) is an anhydrous sugar that can be obtained by pyrolysis of lignocellulosic biomass.[1] This anhydrous carbohydrate can be acylated to obtain carbohydrate fatty acid esters (CFAEs).[2] Here, these compounds were obtained via enzymatic acylation of LG that was commercially obtained (Start BioSci-ence®) and from biomass pyrolysis, with different acyl donors in batch and continuous flow. A comparison was made between a commercial source of LG and the obtained from the enrichment of bio-oil in the formation of CFAEs using two solvents: acetonitrile and cyrene, in batch. For the continuous flow reactions, through the experimental design, it was possible to optimize the reaction conditions, temperature and residence time, obtaining a maximum conversion at 61 °C and 77 min. In addition, there was a productivity gain of up to 100 times in all comparisons made with the batch system. Initial investigation of surfactant properties of obtained products has been carried out by measuring minimum interfacial tension (IFT^{min}). For a mixture of 4- and 2 O-lauryl-1,6-anhydroglucopyran (MONLAU), the minimum interfacial tension (IFT^{min}) obtained was 96 mNm^{-1} and the critical micelle concentration (CMC) was 50 mM. Similar values were obtained for a mixture of 4- and 2-O-palmitoyl-1,6-anhydroglucopyranose, not yet reported in the literature, of 88 mNm^{-1} in 50 mM. For a mixture of 4- and 2 O-oleoyl-1,6-anhydroglucopyranose and 4- and 2-O-estearyl-1,6-anhydroglucopyranose,CMC was higher than 60 mM and IFT^{min} of 141 mNm^{-1} and 102 mNm^{-1}, respectively. Furthermore, promising data were obtained for minimal inhibitory concentration (MIC) and minimal bactericidal concentration (MBC) of MONLAU against *Staphylococcus aureus* strains at 0.25 mM.[3]

Keywords: Levoglucosan, Transesterification, Lipase, Esters, Antibacterial and Biosurfactant.

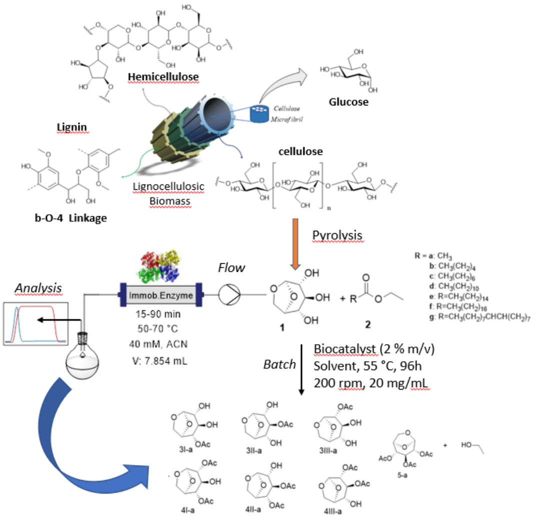

Figure 1:Schematic overview of the lignocellulosic biomass structure and transesterification reaction of levoglucosan with different acyl donors in batch and continous flow.

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Heterotrophic growth of the red microalga *Galdieria Sulphuraria*

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Abstract:

Microalgal biotechnology will be a valuable contribution for achieving industrial sustainability in the near future. The extremophilic red microalga *Galdieria sulphuraria* has considerable potential for sustainable mass cultivation because of its particular growth conditions. This microalga grows heterotrophically at a low pH (pH 2) - thereby considerably reducing the risk of contamination - on a variety of carbon substrates including second generation sources from various industrial waste streams. In particular the use of glycerol, a side product from biodiesel production can be used as an alternative to first generation carbon sources such as glucose. During growth on glycerol, *G. sulphuraria* reaches high cell densities and accumulates high amounts of the polysaccharide glycogen (1). The algal glycogen is unique in its structure and shows potential as a functional ingredient in cosmetic products, sport drinks, and kidney dialysis fluids (2). We report on the heterotrophic growth of several *Galdieria* strains on glycerol and the productivity and structural properties of the glycogen. In addition, we discuss the required upscaled processing steps for a sustainable mass production of the algal glycogen.

Keywords:
Extromophilic, *Galdieria sulphuraria*, glycogen, heterotrophy, microalgae, substrate waste streams, sustainability.

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Flexible Alternatives To Process Intensification For mAb Purification

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Abstract:
A monoclonal antibody (mAb) purification process typically consists of a series of steps: a capture step using Protein A chromatography followed by intermediate and polishing steps using various ion exchange resins and hydrophobic interaction chromatography (HIC) resins. Purification strategies with combined mechanisms of action can allow for fewer chromatography steps to save processing time, thereby making enhancements to overall process economics and efficiency. This case study presents a comparison of a three-step mAb purification process using ion exchange resins post–Protein A capture to a two-step purification using Protein A resin followed by an anionic hydrophobic mixed-mode chromatography resin (Figure 1) . In addition, data from a two-step approach using a calcium affinity cation exchange media after the Protein A step will be presented. The results of both studies using mixed-mode chromatography will show the ability to achieve high-purity product with one fewer unit operation.

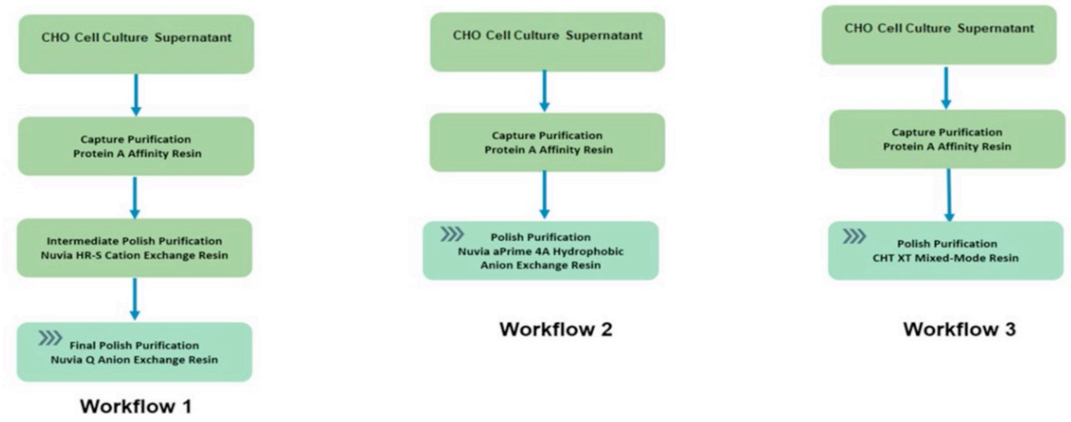

Figure. 1. Overview of the three workflows evaluated.

Bacteria attacking plastic waste

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Abstract:
Intensive exploitation, poor recycling, low repeatable use, and unusual resistance of plastics to environmental and microbiological action result in accumulation of huge waste amounts in terrestrial and marine environments, causing enormous hazard for human and animal life. It is therefore essential to find an ecofriendly solution to this environment hazardous waste. Lately, particular attention has been paid to bacteria and enzymes that could help with the plastic pollution problem. The enzymes discovered util now and used on industrial scale are able to break down polymer of polyethylene terephthalate (PET), found in most consumer packaging but not other types of plastics such as polyethylene (LDPE and HDPE) and polyvinyl chloride (PVC). The objective of this project is to isolate new bacteria able to produce effective enzymes for the degradation of plastics.

A sampling of aged plastic was carried out in a technical landfill to isolate bacteria. Two distinct screening methods were used: the first one is based on the cultivation of bacteria on a mineral medium containing plastic as the only carbon source and the second one consisted of acclimatization over a period of 5 months of microbial populations to pieces of different types of plastic such as PET, PVC, LDPE, or PVC type.

More than 183 strains have been isolated and their potential to degrade different types of plastic has been evaluated on 96 and 24 well plates. An infrared analysis was carried out to evaluate the degradation products and therefore select the best ones. The results showed that among the isolated strains, about twenty have an interesting efficiency for the degradation of PVC and LDPE type plastics. The selected strains have been identified by sequencing and further analyzes are underway to characterize enzymes involved in biodegradation.

Keywords: plastic degradation, bacteria, enzymes, environment, circular economy

High level expression and characterization of extracellular lipase Lip7 from *Yarrowia lipolytica*

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Abstract:

The extracellular lipase from *Yarrowia lipolytica* (YlLip7) was obtained from the genetically modified strain PO1d-LIP7 (with two copies of the gene). High production of YlLip7 protein was obtained by overexpression of the YALI0D19184 gene under strong TEF promoter, in the strain with knocked-out extracellular protease (AEPp). This strategy allowed to prevent the secreted lipase from proteolysis. The purified YlLip7 was found to has its optimal activity at 37 °C and pH 7.5 and retain stable over the pH range of 6.0–10.0. Activity data showed that YlLip7 had an optimal activity for ester p-nitrophenyl octanoate (pNPO, C_8). It was able to hydrolyse esters with longer carbon chain (C_{10}–C_{12}) but the p-nitrophenol palmitate (pNPP, C_{16}) was hydrolysed poorly. The effect of biosurfactants, i.e., surfactin produced by *Bacillus subtilis* #309 and rhamnolipid secreted by *Pseudomonas aeruginosa* #112, on the conformation and activity of YlLip7 was evaluated using spectral methods, surface tension, and enzyme activity assay. The fluorescence spectroscopy analysis confirmed formation of the complexes of YlLip7 with surfactin and rhamnolipid which was also further verified by surface tension measurements. In comparison to the commercial lipases, YlLip7 demonstrated higher tolerance to both biosurfactants and retained more activity after incubation with Tween 20 for up to 24 h. Thus, the YlLip7 with adaptability and stability to broad pH and temperature ranges as well as with high tolerance to lipopeptide and glycolipid biosurfactants is favorable for potential application in various industries including medicine, pharmaceuticals, food and cosmetics.

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Keywords: *Yarrowia lipolytica*; lipase, biosurfactant; lipopeptide; glycolipid, fluorescence spectroscopy, surface tension, biomedical applications.