

## NANOTECH FRANCE 2025 / GAMS 2025 / NANOMATEN 2025

## Joint International Conferences and Exhibition

## 25 - 27 June 2025

## Paris - France

# **Book of Abstracts**

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### Nanotech France 2025 / NanoMatEn 2025 / GAMS 2025

Joint Conferences Program

25 - 27 June 2025, Paris, France

June 25, 2025		
09:00 - 12:00	0 Onsite Participant registration	
09:30 - 10:30	Morning Coffee Break	
	Nanotech France / NanoMatEn / GAMS 2025 Joint Plena	ry session
	Amphithéâtre	
Session's Chairs: Prof. Jacques Jupille, Université Pierre et Marie Curie (UPMC), CNRS Paris, France Prof. Juan Francisco Sánchez Rovo. University of Valencia. Spain		
10:30 - 11:00	From Basic Nanomaterials Physics to Real-world Optoelectronics Applications L. Samuelson	Prof.LarsSamuelson,SUSTech,China/LundUniversity,Sweden/Hexagem AB,Sweden
11:00 - 11:30	Emerging technologies to answer to digitalization demands <b>R.F.P. Martins</b>	Prof.RodrigoFerrãodePaivaMartins,NovaUniversityofLisbon,Portugal
11:30- 12:00	Innovative Micro and Macroporous Polymer Films based on Poly(2,6-dimethyl-1,4-phenylene) oxide: Properties and Applications <b>P. Rizzo</b>	<b>Prof. Paola Rizzo</b> , University of Salerno, <b>Italy</b>
12:00 - 14:00	00 Lunch Break	
Nanotech France / NanoMatEn / GAMS 2025 Joint Session I. A: Nanomaterials Fabrication / Synthesis / Properties		
	Amphithéâtre	
Session's Chairs: Prof. Paola Rizzo, University of Salerno, Italy Dr. Bolli, Villanova University, USA		
14:00 - 14:30	Formation of Nanoaggregates within Deep Eutectic Solvent Based Systems <b>S. Pandey</b>	Prof. Siddharth Pandey, Indian Institute of Technology Delhi, India
14:30 - 15:00	Challenges on the Fabrication of Thermochromic VO2 on Si and Glass Platforms for Multiple Applications <b>F. M. Morales</b> , N. Martin, J. J. Jiménez, A. Casas, R. García and A. J. Santos	<b>Prof. Francisco Miguel</b> <b>Morales Sánchez</b> , University of Cádiz, <b>Spain</b>
15:00 - 15:30	Evidences of out-of-plane trion emission in monolayer WSe2 D. Andrés-Penares and <b>J. F . Sánchez-Royo</b>	<b>Prof. Juan Francisco</b> <b>Sánchez Royo</b> , University of Valencia, <b>Spain</b>
15:30 - 15:45	An Innovative Approach for Fabricating Wrinkled Silver-Based Nanoporous Material S. Asaram Raut, R. Dantinne, A. Chauvin, P. Leclere and <b>D.Thiry</b>	<b>Prof. Damien Thiry</b> , University of Mons, <b>Belgium</b>
15:45 - 16:00	Nanoporous Cu/SiO2 and Zn/SiO2 Hybrid Aerogels and Xerogels: Crystallinity, Porosity and Thermal Stability Al-Z.F. El-Cheikh, W. Kwapinski, M.N. Ahmad, J.J. Leahy and <b>H. El-Rassy</b>	<b>Prof. Houssam Rassy</b> , American University of Beirut, <b>Lebanon</b>
16:00 - 16:30 Afternoon Coffee Break		
Session's Chairs: Prof. Damien Thiry, University of Mons, Belgium Prof. Francisco Miquel Morales Sánchez. University of Cádiz. Spain		
16:30 - 17:00	Salt-assisted coating of MXene on arbitrary polymers L. Zhao, L. Bi, J. Hu, G. Gao, D. Zhang, Y. Li, A. Flynn, R. Wang, L. Liu, Y. Gogotsi and <b>B. Li</b>	<b>Dr. Bo Li</b> , Villanova University. <b>USA</b>

17:00 - 17:15	Synergistic Colloidal System from Gellan Gum and Microalgal Extract: Preliminary Insights into Nano Gelation and Structural Properties <b>F. Sansone</b> , F. Del Prete, F. Fortunato, T. Esposito, R. P. Aquino and T. Mencherini	<b>Prof. Francesca Sansone</b> , University of Salerno, <b>Italy</b>
17:15 - 17:30	Synthesis of mesoporous silica nanoparticles in fluoride medium by spray drying L. Gómez, E. M. Rivero-Buceta, C. Vidaurre-Agut and <b>P.</b> <b>Botella</b>	Dr.PabloBotellaAsuncion,ValenciaPolytechnicUniversity,SpainValencia
17:30 - 17:45	DLC film doped with graphene nanoparticles with very low coefficient of friction in ultra high vacuum condition F. O. Kolawole, E. J. D. M. Pillaca, G. V. Martins, S. K. Kolawole, E. J. Corat and <b>V. J. Trava-Airoldi</b>	Dr. Vladimir Trava- Airoldi, National Institute for Space Research INPE, Brazil
17:45 - 18:00	Nanoscale insight into the functionalization of graphene oxide with porphyrins <b>N. Garro</b> , V. Camús, M. Navarro-Rodríguez, A. Cros and E. Palacios-Lidón	<b>Dr Núria Garro</b> , Univ of Valencia, <b>Spain</b>

June 25, 2025		
Nanotech France / NanoMatEn / GAMS 2025 Joint Session I. B: Nanomaterials Modelling, Characterization and Properties		
	Conference Room Derain 1-2	
Session's Chairs: Prof. Jacques Jupille, Université Pierre et Marie Curie (UPMC), CNRS Paris, France Prof. Lars Samuelson, SUSTech, China/Lund University, Sweden/ Hexagem AB, Sweden Prof. Philippe Heynderickx, Ghent University Global Campus, Rep. of Korea		
14:00 - 14:15	Determination of size distribution of nanomaterials using Field-Flow Fractionation with different detectors <b>H. Kato</b> , A. Nakamura and H. Banno	Dr. Haruhisa Kato, National Institute of Advanced Industrial Science and Tech., Japan
14:15 - 14:30	Theoretical assessment of elastic modulus of carbon nanotubes <b>N. Mallik</b>	<b>Dr. Nilanjan Mallik</b> , Indian Institute of Technology Varanasi, <b>India</b>
14:30 - 14:45	Growth mechanism and some properties of nanostructured graphene on cubic - SiC / Si (001) wafers <b>V. Aristov</b> , O. Molodtsova, S. Babenkov, D. Potorochin, D. Marchenko, A. Locatelli, T. O. Mentes and A. Sala	<b>Prof. Victor Aristov,</b> Deutsches Elektronen- Synchrotron, <b>Germany</b>
14:45 - 15:00	Graphene as a protecting barrier against metal corrosion <b>I. El Hajj</b> , K. Dembélé, B. Laïk and F. Z. Bouanis	<b>Dr. Inass El Hajj</b> , Ecole polytechnique, <b>France</b>
15:00 - 15:15	High-performance room-temperature NO2 gas sensors based on liquid phase exfoliated WS2 ultra-thin films <b>R. Li</b> , E. Ould Maina, K. Dembélé and F.Z. Bouanis	<b>Ms. Ran Li</b> , École Polytechnique, <b>France</b>
15:15 - 15:30	Defect control of graphene using ion beam irradiation and its application to gas sensing. <b>S. Yeo</b> , J. Seo and G. Jeon	<b>Dr. Sunmog Yeo</b> , Korea Atomic Energy Research Institute, <b>Rep. of Korea</b>
15:30 - 15:45	First steps with DFT for plasmon mapping in modified graphene for sensor development <b>A. F. Jiménez González</b> and D. E. Ceballos Herrera	<b>Dr. Ali F. Jiménez</b> <b>González,</b> The National Autonomous University of Mexico, <b>México</b>
15:45 - 16:00	Nanostructured In2O3 Gas Sensors for Ultra-Sensitive H2S Detection at Trace Levels T. Sood and <b>P. Poornesh</b>	<b>Dr Poornesh P</b> , Manipal Institute of Technology, <b>India</b>
16:00 - 16:30	Afternoon Coffee Break	
Session's Chairs: Prof. Victor Aristov, Deutsches Elektronen-Synchrotron, Germany Dr. Haruhisa Kato, National Institute of Advanced Industrial Science and Tech., Japan		
16:30 - 17:00	Nanomaterials for Extreme Environments: From Heteronanotubes to High-Performance Fibres <b>B.M. Maciejewska</b> , R; Schofield, S. Dong, G. Tebbutt, T. Liu, P-Y. Lee and N. Grobert;	Dr. Barbara M. Maciejewska University of Oxford, UK
17:00 - 17:15	FTIR study of Carbonated MgO under Thermal and Plasma treatments <b>T. Elgayyar</b> , F. Azzolina-Jury and F. Thibault-Starzyk	<b>Dr. Taha Elgayyar</b> , University of Caen, <b>France</b>
17:15 - 17:30	Zinc Oxide Aerogel for Water Remediation AI-Z.F. EI-Cheikh, W. Kwapinski, M.N. Ahmad, J.J. Leahy and H. EI-Rassy	Mrs. Al Zahraa Fatima El Cheikh, University of Limerick, Ireland
17:30 -17:45	Poly(2,6-dimethyl-1,4-phenylene)oxide (PPO) nanoporous crystalline films for water remediation <b>D. Riccardi</b> and P. Rizzo	<b>Mr. Domenico Riccardi</b> , Univ. of Salerno, <b>Italy</b>
17:45 - 18:00	Enhanced water desalination via Direct Contact Membrane Distillation using Polyacrylonitrile-derived carbon nanofiber membranes <b>Z. El Charif</b> , A. Hijazi, D. Cornu and M. Bechelany	<b>Ms Zahraa El Charif,</b> Univ Montpellier, <b>France</b>

June 26, 2025		
Nanotech France/ NanoMatEn/ GAMS 2025 Joint Plenary Session II		
	Amphithéâtre	
Session's Chairs: Prof. Juan Francisco Sánchez Royo, University of Valencia, Spain Prof. Ulla Birgitte Vogel, Technical Univ. of Denmark, Denmark		
09:00 - 09:30	A cryogenic energy efficient memory cell for quantum and neuromorphic computing Y. Han, J. Sun, B. Richstein, A. Grenmyr, J. H. Bae, J. Knoch, QT. Zhao and <b>D. Grützmacher</b>	Prof. Detlev Gruetzmacher, Forschungszentrum Jülich, Germany
09:30 - 10:00	Biological mechanisms of actions of nanomaterial-induced respiratory toxicity <b>U. Vogel</b>	<b>Prof. Ulla Birgitte Vogel,</b> National Research Centre for the Working Environment/ Technical Univ. of Denmark, <b>Denmark</b>
10:00 - 10:30	Multifunctional carbon dots for imaging and therapy <b>A. Bianco</b>	<b>Dr. Alberto Bianco</b> , Centre National de la Recherche Scientifique (CNRS), <b>France</b>
10:30 - 11:00	Morning Coffee Break	
11:00 - 11:30	TEM Investigations of Complex Low Dimensional Nanostructures <b>R. Arenal</b>	<b>Dr. Raul Arenal</b> , University of Zaragoza, <b>Spain</b>
11:30 - 12:00	Automated Atomic Scale Data Analysis and Modelling for (Scanning) Transmission Electron Microscopy M. Botifoll, I. Pinto-Huguet and <b>J. Arbiol</b>	Prof. Jordi Arbiol, ICREA / ICN2 / CSIC / BIST, Spain
10.00 11.00		
12:00 - 14:00	Lunch Break	
12:00 - 14:00	Lunch Break NanoMatEn / GAMS Joint Session II. A: Materials and Nanomaterials for Energy / Nanoelectronics/ N	anophotonics
12:00 - 14:00	Lunch Break NanoMatEn / GAMS Joint Session II. A: Materials and Nanomaterials for Energy / Nanoelectronics/ N Amphithéâtre	lanophotonics
12:00 - 14:00	Lunch Break NanoMatEn / GAMS Joint Session II. A: Materials and Nanomaterials for Energy / Nanoelectronics/ N Amphithéâtre Session's Chairs: Prof. Detlev Gruetzmacher, Forschungszentrum Jülich, Prof. Jordi Arbiol, ICREA/ ICN2/ CSIC/ BIST, Spa	lanophotonics Germany in
12:00 - 14:00 14:00 - 14:30	Lunch Break NanoMatEn / GAMS Joint Session II. A: Materials and Nanomaterials for Energy / Nanoelectronics/ N Amphithéâtre Session's Chairs: Prof. Detlev Gruetzmacher, Forschungszentrum Jülich, Prof. Jordi Arbiol, ICREA/ ICN2/ CSIC/ BIST, Spa Functionalized Nanodiamond Fluids in Transformers Thermal Management – A CFD Modeling Study P. Swiecichowski and E. Languri	anophotonics Germany in Prof. Ethan Languri, Tennessee Tech University, USA
12:00 - 14:00 14:00 - 14:30 14:30 - 15:00	Lunch Break         NanoMatEn / GAMS Joint Session II. A:         Materials and Nanomaterials for Energy / Nanoelectronics/ N         Amphithéâtre         Session's Chairs:         Prof. Detlev Gruetzmacher, Forschungszentrum Jülich, Prof. Jordi Arbiol, ICREA/ ICN2/ CSIC/ BIST, Spa         Functionalized Nanodiamond Fluids in Transformers Thermal Management – A CFD Modeling Study P. Swiecichowski and E. Languri         Materials and Surface Engineering for Outdoor Electrical Insulation A. Milionis, A. Leal-Ayala, P. Meier and D. Hohl	Germany in Prof. Ethan Languri, Tennessee Tech University, USA Dr. Athanasios Milionis, ABB Switzerland Ltd., Switzerland
12:00 - 14:00 14:00 - 14:30 14:30 - 15:00 15:00 - 15:15	Lunch Break         NanoMatEn / GAMS Joint Session II. A:         Materials and Nanomaterials for Energy / Nanoelectronics/ N         Amphithéâtre         Session's Chairs:         Prof. Detlev Gruetzmacher, Forschungszentrum Jülich, Prof. Jordi Arbiol, ICREA/ ICN2/ CSIC/ BIST, Spa         Functionalized Nanodiamond Fluids in Transformers         Thermal Management – A CFD Modeling Study         P. Swiecichowski and E. Languri         Materials and Surface Engineering for Outdoor Electrical Insulation         A. Milionis, A. Leal-Ayala, P. Meier and D. Hohl         Development of High Performance Polydimethylsiloxane- Multi-walled Carbon Nanotubes (PDMS-MWCNTs) Nanocomposites for Triboelectric Nanogenerator Applications         M. Ahmed, A.M. K. Esawi and M. Arafa	Germany         in         Prof. Ethan Languri,         Tennessee         University, USA         Dr. Athanasios Milionis,         ABB         Switzerland         Ltd.,         Switzerland         Ms. Manal Ahmed, The         American University in         Cairo, Egypt
12:00 - 14:00 14:00 - 14:30 14:30 - 15:00 15:00 - 15:15 15:15 - 15:30	Lunch Break         NanoMatEn / GAMS Joint Session II. A:         Materials and Nanomaterials for Energy / Nanoelectronics/ N         Amphithéâtre         Session's Chairs:         Prof. Detlev Gruetzmacher, Forschungszentrum Jülich, Prof. Jordi Arbiol, ICREA/ ICN2/ CSIC/ BIST, Spa         Functionalized Nanodiamond Fluids in Transformers         Thermal Management – A CFD Modeling Study         P. Swiecichowski and E. Languri         Materials and Surface Engineering for Outdoor Electrical Insulation         A. Milionis, A. Leal-Ayala, P. Meier and D. Hohl         Development of High Performance Polydimethylsiloxane- Multi-walled Carbon Nanotubes (PDMS-MWCNTs) Nanocomposites for Triboelectric Nanogenerator Applications         M. Ahmed, A.M. K. Esawi and M. Arafa         Sunlight-Driven Nanostructured Polymer Coatings for Energy-Efficient Smart Surfaces         P. Das, L. Charlton and A. J. C. Semiao	Germany         in         Prof. Ethan Languri,         Tennessee Tech         University, USA         Dr. Athanasios Milionis,         ABB Switzerland Ltd.,         Switzerland         Ms. Manal Ahmed, The         American University in         Cairo, Egypt         Dr. Pritam Das, The         University of Edinburgh, UK
12:00 - 14:00 14:00 - 14:30 14:30 - 15:00 15:00 - 15:15 15:15 - 15:30 15:30 - 15:45	Lunch Break         NanoMatEn / GAMS Joint Session II. A:         Materials and Nanomaterials for Energy / Nanoelectronics/ N         Amphithéâtre         Session's Chairs:         Prof. Detlev Gruetzmacher, Forschungszentrum Jülich, Prof. Jordi Arbiol, ICREA/ ICN2/ CSIC/ BIST, Spa         Functionalized Nanodiamond Fluids in Transformers         Thermal Management – A CFD Modeling Study         P. Swiecichowski and E. Languri         Materials and Surface Engineering for Outdoor Electrical Insulation         A. Milionis, A. Leal-Ayala, P. Meier and D. Hohl         Development of High Performance Polydimethylsiloxane- Multi-walled Carbon Nanotubes (PDMS-MWCNTs) Nanocomposites for Triboelectric Nanogenerator Applications         M. Ahmed, A.M. K. Esawi and M. Arafa         Sunlight-Driven Nanostructured Polymer Coatings for Energy-Efficient Smart Surfaces         P. Das, L. Charlton and A. J. C. Semiao         Effect of electron-phonon interaction on thermoelectric properties through DNA chains         J. H. Ojeda, Santanu K. Maiti, D. Laroze, G. Eramo and P. A. Orellana	Germany         in         Prof. Ethan Languri,         Tennessee Tech         University, USA         Dr. Athanasios Milionis,         ABB Switzerland Ltd.,         Switzerland         Ms. Manal Ahmed, The         American University in         Cairo, Egypt         Dr. Pritam Das, The         University of Edinburgh, UK         Prof Judith H. Ojeda         Silva, Pedagogical and         Technological University of         Colombia, Colombia

June 26, 2025		
Nanotech France / GAMS 2025 Joint Session II. B: Nano for life science and Medicine		
Conference Room Derain 1-2		
Session's Chairs: Dr. Alberto Bianco, Centre National de la Recherche Scientifique (CNRS), France Dr. Pablo Botella Asuncion, Valencia Polytechnic University, Spain Dr. Vida A. Dennis, Alabama State University. USA		
14:00 - 14:30	Harnessing Nanotechnology and Plasmonics at the Frontiers of Biomedical Diagnostics <b>T. Vo-Dinh</b>	<b>Prof. Tuan Vo-Dinh</b> , Duke University, <b>USA</b>
14:30 - 15:00	Scalable Microfluidic Synthesis of PEGylated Liposomes for Drug Delivery and Cosmetic Applications S. Akar, S. Fardindoos and <b>M. Hoorfar</b>	<b>Prof. Mina Hoorfar,</b> University of Victoria, <b>Canada</b>
15:00 - 15:15	Molecular Dynamics in Nanomedicine: From Molecular Insights to Functional Design <b>P. Siani</b> , G. Frigerio, E. Donadoni and C. Di Valentin	Dr. Paulo Siani Paulo, University of Milano- Bicocca, Italy
15:15 - 15:30	Mycosynthesis, Characterization, and Mosquitocidal Activity of Silver Nanoparticles Fabricated by Aspergillus niger Strain M.A. Awad, A.M. Eid, T.M. Y. Elsheikh, Z.E. Al-Faifi, N. Saad, M.H. Sultan, S. Selim, <b>A.A. Al-Khalaf</b> and A. Fouda	Prof. Areej Al-Khalaf, Princess Nourah bint Abdulrahman Univ, Saudi Arabia
15:30 - 15:45	A New bone nano-hemostatic agent with antibacterial activity <b>M. Salah</b>	<b>Dr. Mohammed Salah</b> , King Saud Univ., <b>Saudi</b> <b>Arabia</b>
15:45 - 16:00	Multifunctional properties of Dy <sub>2</sub> O <sub>3</sub> -Doped ZnO nanoparticles: Optical, dielectric, and antibacterial performance <b>T. Almuatiri Atia</b> , R. Hamdi, E. Kotb and A. ben Ali	Ms. Taghreed Almuatiri Atia, Qassim University, Saudi Arabia
16:00 - 16:30	Afternoon Coffee Break	
Session's Chairs: Prof. Imran Saleem, Liverpool John Moores University, UK Prof. Mina Hoorfar, University of Victoria, Canada		
16:30 - 17:00	Mn-Doped Carbon Dots as MRI Contrast Agents: Insights from Phantom Studies toward Neuroimaging Use <b>C.M. Uritu</b> , S.I. Filipiuc, A. Coroaba, A. Fifere, I. Spiridon, N.L. Marangoci and B.I.Tamba	<b>Dr. Cristina Mariana Uritu</b> Grigore T. Popa University of Medicine and Pharmacy of Iasi, <b>Romania</b>
17:00 - 17:15	Development of stable biofuntionalize PET membranes with bioactive binding points for potential application in cell culturing devices <b>D. Stan</b> , L.A. Bocancia-Mateescu, A.C. Mirica and S. Mocanu	<b>Dr. Dana Stan</b> , DDS Diagnostic SRL, <b>Romania</b>
17:15 - 17:30	Sol-Gel Synthesis of Silica-based Biomaterials containing Rosmarinic Acid and Polyethylene Glycol <b>F. Barrino</b> , F. Giuliano and C. Dispenza	<b>Dr. Federico Barrino</b> , University of Palermo, <b>Italy</b>
17:30 - 17:45	Non-Invasive Label-Free Electrical and Optical Parrallel Recordings of Electrophysiological Action Potentials of hiPSC Cardiomyocytes <b>J. Hurtaud</b> , A. Boschi, G. Iachetta, M. Dipalo and F. De Angelis	<b>Dr. Julien Hurtaud</b> , Italian Institute of Technology, <b>Italy</b>
17:45 - 18:00	Homogenously-sized PLGA-encapsulated chlamydial protein is effi-ciently delivered into dendritic cells by activating the caveolin endo-cytosis pathway to boost innate immune responses <b>V.A. Dennis</b> , R. Sahu, A.C.N. Sipowe, V. Tadjuidje and L. Gildea	<b>Dr. Vida A. Dennis</b> , Alabama State University, <b>USA</b>

June 27, 2025		
Nanotech France/ GAMS 2025 Joint Session III: Nano for life science and Medicine		
Session's Chairs: Prof. Mina Hoorfar, University of Victoria, Canada Prof. Francesca Sansone, University of Salerno, Italy		
	Conference Room Derain 1-2	
09:00 - 09:30	Remote Cellular Manipulation Using Magnetic Nanoparticles for Tissue Engineering and Stimulation <b>C. Wilhelm</b>	<b>Prof. Claire Wilhelm</b> , Paris Diderot University, <b>France</b>
09:30 - 10:00	Unlocking Non-parenteral Routes: Nanocarrier Systems for Biological Therapeutics I. Saleem	<b>Prof. Imran Saleem</b> , Liverpool John Moores University, <b>UK</b>
10:00 - 10:30	Morning Coffee Break	
10:30 - 10:45	Fish Scales Derived Bioapatite and it's Nanotoxicity on Development of Zebrafish Embryo <b>R. Kaur</b> and Rishu	<b>Dr. Ravneet Kaur</b> , Panjab University, <b>India</b>
10:45 - 11:00	Novel Nanoformulations for Breast Cancer Drug Delivery Nanocarriers, Bone Regeneration Scaffolds and Industrial Applications <b>W. Mamdouh</b> , N. M. Elbaz, L. Ziko, R. Siam, N. S.Farrag, H.A.El-Sabagh, A. M. Al-mahallawi, A. M.Amin and A. AbdEl- Bary	<b>Prof. Wael Mamdouh</b> , The American University in Cairo, <b>Egypt</b>
11:00 - 11:15	1,8-Cineole-loaded Chitosan Nanoparticles: Optimization via Box-Behnken Design, Characterization, Release Kinetics, and Dual In Vitro–In Silico Evaluation Against HeLa Cancer Cell Line <b>A. Shetta</b> , C.D. Lorenz, and W. Mamdouh	<b>Dr. Amro Shetta</b> , The American University in Cairo, <b>Egypt</b>
11:15 - 11:30	Surface-Modified Drug Nanoparticles in Reinforced Hydrogel Matrix: A Sustainable Approach for Diabetic Wound Management <b>Z. Zhang</b> and W. Wen	<b>Ms. Ziyi Zhang</b> , The Hong Kong University of Science and Technology, <b>China</b>

### **Posters Sessions**

### June 25 and 26, 2025

N.	Title	Author / Affiliation / Country
1.	Morphological and Structural Engineering of Niobium Selenide Nanostructures via Chemical Vapor Transport <b>N. Abdelrahman</b> , S; Froeschke, A. Popov, S. Schiemenz, D. Wolf, R; Giraud, A. Soliman, B. Büchner, M. Mertig and S. Hampel	Mrs. Nour Abdelrahman, Leibniz Institute for Solid State and Materials Research, Germany
2.	Fluorescent half-salen phenoxy-imine zinc complexes to reveal exogenous and endogenous H2S <b>A. Trerotola</b> and M. Strianese	<b>Mr. Alessio Trerotola</b> , Univ. of Salerno, <b>Italy</b>
3.	Very High Efficacy In Vitro Terapy of Human Melanoma Cancer by Superparamagnetic Hyperthermia with Magnetite-Hydroxypropyl- Gamma-Cyclodextrin Nanoparticles <b>C. Caizer</b> , I.S. Caizer-Gaitan, C.G. Watz, Z. Crainiceanu and C.M. Soica	<b>Prof. Costica Caizer</b> , West University of Timisoara, <b>Romania</b>
4.	Targeted Doxorubicin delivery and release within breast cancer environment using PEGylated chitosan nanoparticles labeled with monoclonal antibodies" <b>O. Helmi</b> , F. Nabil and W. Mamdouh	<b>Mr. Omar Helmi</b> , American University in Cairo, <b>Egypt</b>
5.	Inhibitory effect on retinal neovascularization of gold nanodisks optically tuned for optical coherence tomography <b>J. Hun Kim</b> and T. Geol Lee	Prof. Jeong Hun Kim, National University Hospital Seoul, Rep. of Korea
6.	A measurement method for assessing the dimensions of shape patterns utilizing silver-nano inks in printed electronics <b>C.H. Kim</b> , D.S. Kim and J. Lee	Prof. Chung-Hwan Kim, Chungnam National University, Rep. of Korea
7.	Poly(butylene succinate) (PBS) films composites with carbon black <b>A. Erbaggio</b> , M.R. Acocella, P. Lamberti, V. Tucci and P. Rizzo	Ms. Angela Erbaggio, University of Salerno, Italy
8.	CuO Nanoparticles-Decorated Femtosecond Laser-Irradiated WS2– WO3 Heterojunctions to Realize Selective H2S Gas Sensors JH. Kim	<b>Prof. Jae Hun Kim</b> , Inha University, <b>Rep. of Korea</b>
9.	Comprehensive Kinetic Modeling and DFT Analysis of Cationic and Anionic Dye Photocatalytic Degradation: Insights for Green Chemistry and Water Treatment Technologies A. Ranibari and <b>P.M. Hevnderickx</b>	<b>Prof. Philippe Heynderickx</b> , Ghent University Global Campus, <b>Rep. of Korea</b>
10.	Evaluating the Catalytic Performance of Mo3P for the Hydrogen Evolution Reaction in Alkaline Media <b>R. Oriňaková</b> , A. Gubóová, M. Strečková and M. Paračková	<b>Prof. Renáta Oriňaková</b> , Pavol Jozef Šafárik University in Košice, <b>Slovakia</b>
11.	Carrageenan as an Ecological Binder for Sulfur-Based Nanostructured Electrodes for Li-S batteries <b>A. Straková Fedorková</b> , V. Niščáková, D. Zalka, N. Podrojková and I. Šišoláková	<b>Prof. Andrea S. Fedorkova</b> , Pavol Jozef Šafárik University in Košice, <b>Slovakia</b>
12.	Effect of acid etching on the supercapacitive performance of electroless Ni-B coatings <b>M. Czagany</b> , G. Meszaros and P. Baumli	<b>Dr. Mate Czagany</b> , University of Miskolc, <b>Hungary</b>
13.	Interfacial behavior between the electrolyte and the electrode <b>P. Baumli</b> , M. Czagany and M. Khairi	<b>Prof. Peter Baumli</b> , University of Miskolc, <b>Hungary</b>
14.	The impact of copper anodization and microwave plasma treatment on energy storage applications <b>A.Sarra</b> , R. Michael and B. Ibtissem	<b>Mrs. Sarra Aoun</b> , Univ. Sorbonne Paris Nord, <b>France</b>
15.	Use of ceramic oxides to reduce erosion of wind turbines due to solid particle impact. L.E. Ramirez Pena, C.M. Garcia and J.S. Hernandez	<b>Mr. Luis E. Ramirez Pena</b> , ESFM-IPN, <b>Mexico</b>
16.	Development of nanobiocatalytic systems toward the valorization of agri- food wastes M. Patila,, A. Alatzoglou, P.E. Athanasiou, S. Spyrou, V. Tolis, F. Luka, P. Kyriakou, A. Polydera and <b>H. Stamatis</b>	<b>Prof. Haralambos Stamatis</b> , University of Ioannina, <b>Greece</b>
17.	Development of Chymosin-Based Nanobiocatalyst through Immobili- zation on High Quality Few-Layer Bio-Graphene C. Alatzoglou, M. Patila, A. Skonta, M. Bellou, S.Spyrou, P. Athanasiou, K. Spyrou, D. Gournis, <b>A.C., Polydera</b> , P. Katapodis, D. Houhoula and H. Stamatis	<b>Dr. Angeliki Polydera,</b> University of Ioannina, <b>Greece</b>

## Nanotech France / NanoMatEn / GAMS 2025 Joint Plenary session

## From Basic Nanomaterials Physics to Real-world Optoelectronics Applications

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### Abstract:

Nanoscale Materials Science is driven both by curiosity for fundamental materials physics, and by the frequently occurring realization of applications enabled by this field of research. One special such area is that of nanowires, a field that exploded about 20 years ago, leading to the availability of ideal one-dimensional materials enabling novel physics studies as well as applications in electronics, photonics and of many other areas [1]. I will zoom in on the case of GaN-based LEDs, leading up to a description of how this rechnology has developed into the expected ultra-small microLEDs as needed for Augmented Reality (AR) applications.

For large-sized LEDs, it is still only Blue and Green that is efficiently generated by directly emitting III-Nitride devices, while the Red is primarily achieved from AlGaInP/GaAs. However, for pixel sizes approaching 10 µm, and below, top-down processing of AlGaInP wafers lead to un-acceptable defects killing the efficiencies. Although the III-Nitride system is less prone to efficiency killed by processing induced defects and carrier diffusion, it is still primarily for the Blue and Green where the GaN-based devices function well. This is due to the large difference in lattice-constant of Red-emitting InGaN quantum wells containing > 35% Indium and the substrate of GaN. We have been developing a very different approach where we replace the substrate of GaN with a relaxed c-oriented substrate of InGaN with In-concentrations up to 20%, by which the lattice mis-match becomes similar as for very efficient Blue QWs on GaN [2,3]. I will here report how we use bottom-up crystal growth, inheriting methods from seeding of GaN nanowires, resulting in extended and dislocation-free platelets of InGaN, freely separated from the GaN substrate and the growth mask. On top of these platelets we form the entire micro/nanoLED structure giving IQE- values exceeding 60% also for saturated Red, for lateral device sizes of less than 1 µm.



**Keywords**: Light-emitting diodes, LEDs, GaN, Gallium-Nitride, microLEDs, lattice mis-match, pixel-sizes, Displays, Augmented Reality, Optical switching.

**Figure 1**: SEM-images of arrays and individual InGaN microLEDs formed by epitaxial bottomup self-assembly, seeded by a GaN nanowire seed developed into dislocation-free and relaxed InGaN pyramidal structure.

Acknowledgment: I want to acknowledge key contributions from colleagues, students and Hexagem R&D people.

- Barrigon, E., Heurlin, M., Bi, Z., Monemar, B., Samuelson, L. (2019) Synthesis and Applications of III-V Nanowires, *Chem. Rev.* 2019, 9170-9220.
- 2. Bi, Z., et al. (2019) InGaN Platelets: Synthesis and Applications toward Green and Red Light-Emitting Diodes, *Nano Lett* 19, 2832.
- 3. Bi, Z., Gustafsson, A., Samuelson, L. (2023) Bottom-up approaches to microLEDs emitting red, green and blue light based on GaN nanowires and relaxed InGaN platelets, *Chin. Phys. B*, Vol. 32(1), 018103

## Emerging Technologies to Answer to Digitalization Demands

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### Abstract:

In the current digital era, as the world is growing up with smart technology, at the same time our planet is drowning with materials scarcity, a huge number of unrecycled waste and environmental pollution. The world is facing challenges against rapid climate continuous ecological changes and disturbances, caused by the revolutionary growth in socio-economic developments with the fastest growing trend in smart electronics, plastic-based products, and the continuous dependence on non-recyclable raw materials. On the other hand, a huge significant progress in IoT and wearable smart electronics systems is demanding very high-resolution displays of the communication interface and the use of green technologies, exploiting emerging devices beyond silicon, most of them at a nanoscale basis. Moreover, energy is required to foster and power all these demands.

This is a way forward to minimize the electronic waste (e-waste) caused by the everincreasing number of disposable electronic devices.

In that context, we aim to contribute to future green products, green powered, and make social awareness of green and sustainable technology, which could revolutionize the industry and society both with new business approaches with smart sustainable lifestyles.

**Keywords**: responsible electronics; flexible electronics; transparent electronics; sustainable electronics



Figure 1. Eco-strategies for next generation materials engineering and applications

### **Reference:**

D. Nunes, A. Pimentel, P. Barquinha, M. Mendes, J. Coelho, H. Almeida, E. Fortunato, R. Martins, Flexible devices based on metal oxides: achievements and prospects, in Metal oxide series, editor G. Korotecenkov, 2025, ISBN 04432165689780443216565

## Innovative Micro and Macroporous Polymer Films based on Poly(2,6dimethyl-1,4-phenylene) oxide: Properties and Applications

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Abstract: In this communication, structural features of Nanoporous Crystalline (NC) phases of two relevant commercial polymers as syndiotactic polystyrene (s-PS) and poly(2,6-dimethyl-1,4-phenylene)oxide (PPO) will be reported (1-2). Moreover, a focus on the extraordinary fast kinetics of guest uptake from PPO NC films, (from a few up to hundred microns of thickness) if prepared by suitable co-crystallization procedures, will be presented (3-4).

A general method to achieve high surface area (HSA) PPO films (up to 620 m2/g), will be also reported (3-4). Because of their extremely fast kinetics of pollutant uptakes, associated with high thermal and mechanical stability, these new HSA NC PPO films are expected to find many applications in pollutant remediation, molecular separations, and molecular sensors. Moreover, we also found crystallization conditions leading to HSA PPO films with transparency and toughness comparable with those for amorphous films (Figure 1). These HSA, transparent, and tough NC PPO films are expected to be suitable for many applications where these properties are needed

Finally, an innovative method to realize PPO films with hydrophilic sulfonated amorphous phase and physically crosslinking hydrophobic crystalline phase as well as their possible applications as molecular sensors, will be presented (5-6).



**Figure 1**: Digital photos of PPO films with a thickness of 50 mm (A-D). PCE sorption kinetics at p/p0 = 0.01 and 35°C for different PPO films

**Keywords**:Nanoporous crystalline phases, Transparent and Flexible films, Pollutant sorption, Molecular sensors.

### **References:**

- G. Guerra, C. Daniel, P. Rizzo et. Al. J. Polym. Sci. Part B: Pol. Phys. 2012, 50, 305-322.
- 2. P. Rizzo, V. Vitale, C. Gallo, O. Tarallo, G. Guerra *Polymer* 2019,167, 193-201.
- 3. A. Cozzolino, B. Nagendra, P. Rizzo, G. Guerra. *Eur. Polym. J.* 2022, 164,110976.
- B. Nagendra, S. Salman, C. Daniel, P. Rizzo, G. Guerra Mater. Adv., 2023, 4,881-89.
- B. Nagendra, S. Salman, H.P. Bloch, C. Daniel, P. Rizzo, R. Fittipaldi, G. Guerra ACS Appl. Polym. Mater. 2023,5,3489–3498.
- P. Rizzo et. Al. Journal of Photochemistry & Photobiology, A: Chemistry, 2025, 115993

### Acknowledgements:

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Nanotech France / NanoMatEn / GAMS 2025 Joint Session I. A: Nanomaterials Fabrication / Synthesis / Properties

## Formation of Nanoaggregates within Deep Eutectic Solvent Based Systems

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### Abstract:

The formation of nanoaggregates within deep eutectic solvents (DESs) represents а groundbreaking approach in the field of sustainable nanotechnology and green chemistry. DESs, usually composed of H-bond donors (HBDs) and H-bond acceptors (HBAs), possess unique properties such as low volatility, biodegradability, and tunable physicochemical characteristics, providing an ideal medium for the self-assembly of nanoaggregates. These aggregates, including micelles, reverse micelles, and vesicles, are influenced by DES polarity and composition, enabling applications in drug delivery, nanomaterial synthesis, catalysis, and biophysics.

Nanoaggregate formation is facilitated through two processes: surfactant-assisted and surfactantfree self-assembly. Surfactant-assisted systems leverage traditional surfactants, with aggregation driven by hydrophobic interactions, electrostatic forces, and H-bonding. DESs enhance surfactant solubility, reduce critical micelle concentration (cmc), and enable the stabilization of distinct nanostructures, including elongated and cylindrical micelles, depending on the surfactant and DES composition. On the other side, surfactant-free systems utilize the amphiphilic nature of DES components to stabilize aggregates without conventional surfactants. Within surfactant-free systems, amphi-solvent facilitates the formation of stable structures by reducing free energy at the interfaces and mesoscale aggregates are stabilized by weak interactions, such as H-bonding or van der Waals forces.

By utilizing the synergy between DESs and surfactants or amphi-solvents, the properties of nanoaggregates, such as size, morphology, and stability, can be finely tuned. These versatile systems align with green chemistry principles, paving the way for innovations in sustainable nanostructure design for pharmaceutical, environmental, and industrial applications.

**Keywords**: nanoaggregation, micelles, deep eutectic solvents (DESs), surfactant aggregation, surfactant-free microemulsion.

- R. G. Lakshmi.; M. Ajay.; P. Nilanjan, Choline chloride-Urea based deep eutectic Solvent: Characterization, interfacial behavior and Synergism in binary (surfactant) systems, *Chem Phys.* 2025, 588, 112496.
- M. Basu.; P. A. Hassan.; B. Sandeep, Shelar Modulation of surfactant self-assembly in deep eutectic solvents and its relevance to drug delivery-A review. J. Mol. Liq. 2023, 375, 121301.
- Y. Han.; N. Pan.; Li. D.; S. Liu.; B. Sun.; J. Chai.; Li. Dejie, Formation Mechanism of Surfactant-Free Microemulsion and a Judgment on Whether It Can Be Formed in One Ternary System. J. Chem. Eng. 2022, 437, 135385–11.

### Challenges on the Fabrication of Thermochromic VO<sub>2</sub> on Si and Glass Platforms for Multiple Applications

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### Abstract:

This presentation aims to describe as a summary, the advances we have performed during the last few years on the development of VO<sub>2</sub> by our original and patented method of oxidizing metallic V, instead of the more common way of reducing V<sub>2</sub>O<sub>5</sub>. In a first stage, we set this proccesss up by the reaction of V nanoparticles with air inside open tubes heated by SiC resistances to achieve powders with a high load of vanadium dioxide [1,2]. The advantage of this method is that we do not use overpressures or high-vaccumms, or any special gas or reactive, just it is done at ambient conditions, but the key point is the high control of both fast heating (~50°C/s) and maintenance of a constant temperature for the precursors (in the 400-700°C range). Based on this knowledge, we could later adapt our recipes to transform in an efficient way, 50 to 500 nm layers of V oblique nanocolums into thin films of vanadium oxides mixes with a predominance of the VO<sub>2</sub> phase. The vanadium placed in this manner acquire a nanoporous structure that eases the homogeneous oxidation through the layers, because of their high surfaceto-volume ratios, thanks to its physical vapor deposition by glancing-angle sputtering. These structures have been oxidized in CAR (calm air heated by resistances) but also in AFIR (air flow heated by infrared lamps). Another variation of these formats has been to integrate dopants as W, Ta or Nb into the V-AOD matrixes. Thus, any combination have their own optimal recipe and lead to diferent optical and electronic properties of every reached VO<sub>2</sub>-based films. In this way, thermochromic films were demonstrated and improved more and more in a chronological order that complies: (i) CAR for 700 nm [3]and 100-300 nm V-OAD [5] on silicon substrates; and (ii) CAR for 12.5-25 nm V-compact [4], and for [6] 50 nm and [7] 25/100 nm V-OAD, and V:W, V:Ta, and V:Nb, on glass substrates. On a last stage, the best results ever obtained in this contexts, and in general compared with the state of the art VO<sub>2</sub> layers growh by other much more sophisticated techniques, are achieved for zigzag V-OAD layers [8,9] (Fig. 1), using CAR and AFIR oxidations, respectively, that allowed getting thickness uniform pure dioxide at a medium scale industrializable templates. The structural and compositional characterizations have been multitechnique, mainly based on TEM, XRD and Raman spectroscopy. While glass supports are researched for smart windows applications, Si is envisaged for IR filters and broadband photodetectors, so optical vis-NIR transmission are presented for variable temperature, while resistivity values ares shown for variable temperature or irradiation of different wavelength sources. In all cases when good quality VO<sub>2</sub> is present, an abrupt metal-toinsulator transition is observed for temperature, voltage or irradiance variations.



Figure 1: 100 nm V zig-zag on Si; surface of an optimized 180 nm poly-crystalline  $VO_2$  layer after oxidation; and its optical responses on Si [9].

- 1. Chem. A Eur. J. 27 (2021) 16662–16669. doi:10.1002/chem.202102566.
- 2. Nanomaterials. 12 (2022) 1471.doi:10.3390/nano12091471.
- 3. Surf. Interfaces. 27 (2021) 101581. doi:10.1016/j.surfin.2021.101581.
- 4. Surf. Interfaces. 34 (2022) 102313. doi:10.1016/j.surfin.2022.102313.
- 5. Chem. Mater. 35 (2023) 4435–4448. doi:10.1021/acs.chemmater.3c00613.
- 6. Energy Build. 285 (2023) 112892. doi:10.1016/j.enbuild.2023.112892.
- Sol. Energy Mater. Sol. Cells. 254 (2023) 112253. doi:10.1016/j.solmat.2023.112253.
- Constr. Build., 419 (2024) 135472. doi:10.1016/j.conbuildmat.2024.135472.
- 9. Appl. Surf. Sci. Adv. 25 (2025) 100692. doi:10.1016/j.apsadv.2025.100692.

### Evidences of out-of-plane trion emission in monolayer WSe<sub>2</sub>

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#### Abstract:

Manipulation of light emitted by twodimensional semiconductors grounds forthcoming technologies in the field of onchipcommunications [1-3]. However, these technologies require from the so elusive out-ofplane photon so The urces to achieve anefficient coupling of radiated light into planar devices [4-10]. Here we propose a versatile spectroscopic method that enables theidentification of the outof-plane component of dipoles. The method is based on the selective coupling of light emitted by in-plane andout-of-plane dipoles to the whispering gallery modes of spherical dielectric microresonators, in close contact to them. We have applied this method to demonstrate the existence of dipoles with an out-of-plane orientation in monolayer WSe2 at room Micro-photoluminescent temperature [11]. measurements, numerical simulations based on finite element methods, and ab-initio calculations have identified trions as the source responsible for this out-of-plane emission, opening new routes for realizing on-chip integrated systems with applications in information processing and quantum communications. For instance, results reported here would allow to identify at any temperature, potential sources for radially polarized light in monolayer transition-metal dichalcogenides, which may have applications in imaging, phase modulation, and diffractive optics, due to the cylindrical symmetry of their light. Also, this methodopens up new routes for the realization of planar devices efficiently exploiting the fundamental properties of atomically thin materials. Finally, iot should be mentioned that the proposed technique does not require magnetic fields and can be easily implemented, makingit accessible, versatile, and technologically relevant.

**Keywords**: optical properties, two-dimensional semiconductors, optoelectronic applications.



**Figure 1**: Illustration of the experimental system to evidence light-matter coupling giving rise to

whispery gallery modes in dielectric microspheres dropped on 2D semiconductors. **References:** 

- 1. R. Won, et al. Nat. Photonics 4, 882 (2010).
- S. H. Bae, et al., Nat. Mater. 18, 550–560 (2019).
- Z. Jia, et al., ACS Appl. Mater. Interfaces 11, 20566–20573 (2019).
- 4. X. Mu, et al., Appl. Sci. 10, 1538 (2020).
- 5. T. Ren, et al., J. Appl. Phys. 125, 230901 (2019).
- 6. Z. Wang, et al., Opt. Lett. 41, 4146–4149 (2016).
- 7. Y.C. Jun, et al., Opt. Express 17, 7479 (2009).
- 8. N. R. Verhart, et al., Opt. Express 22, 19633 (2014).
- M. I. Davanco, et al., Opt. Express 17, 10542 (2009).
- 10. L. Liebermeister, et al. Appl. Phys. Lett. 104, 031101 (2014).
- 11. D. Andrés-Penares, et al., Commun. Mater 2, 52 (2021).

## An Innovative Approach for Fabricating Wrinkled Silver-Based Nanoporous Material

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### Abstract:

Wrinkled nanoporous surfaces exhibit remarkable properties that make them suitable for a wide range of applications.<sup>1</sup> However, their development is hindered by limitations in the current synthesis methods for these complex materials. In this work, we introduce an innovative plasma-derived technique for fabricating silver-based nanoporous wrinkled surfaces. By depositing a magnetron-sputtered Ag-Al alloy layer onto a liquid plasma polymer film (PPF), we exploit the spontaneous wrinkling phenomenon that occurs in bilayer systems comprising a soft layer and a stiff layer.<sup>2</sup>

wrinkled surface is subsequently The nanostructured through dealloying-selective etching of the less noble element in the alloyresulting in the formation of a nanoporous structure that retains the wrinkled morphology as illustrated in Figure 1. Notably, the PPF thickness influences the wrinkle amplitude while maintaining a constant wavelength. This behavior is attributed to the pinning of the metal layer to the silicon substrate. Furthermore, increasing dealloying time enlarges the nanopores but reduces the wrinkle amplitude. This behavior is explained by the shrinkage of the metal layer during dealloying, which induces tensile strain.

Our comprehensive analysis demonstrates the potential of our strategy for fabricating nanostructured patterns with customizable dimensions.

**Keywords**: dealloying, nanomaterial synthesis, nanoporous, plasma polymerization, wrinkling



**Figure 1**: Plane-view SEM image of a wrinkled silver-based nanoporous surface.

- Zhang, L.; Lang, X.; Hirata, A.; Chen, M. (2011) Wrinkled Nanoporous Gold Films with Ultrahigh Surface-Enhanced Raman Scattering Enhancement, ACS Nano, 5, 4407-4413.
- Thiry, D., Vinx, N., Damman, P., Aparicio, J.A., Tessier, P.Y., Moerman, D., Leclère, P., Godfroid, T., Desprez, S., Snyders, R., (2020), The Wrinkling concept applied to plasma-deposited polymer-like thin films: A promising method for the fabrication of flexible electrodes, *Plasma Process. Polym.*, 17, e2000119.

## Nanoporous Cu/SiO<sub>2</sub> and Zn/SiO<sub>2</sub> Hybrid Aerogels and Xerogels: Crystallinity, Porosity, and Thermal Stability

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### Abstract:

Metal oxide aerogels are highly porous materials with large surface areas, high porosity, and low density. These aerogels are obtained via the lowtemperature sol-gel process followed by drying under supercritical conditions. The drying technique largely attenuates the capillary stress responsible for the network compression, its shrinkage, and subsequently the loss of its porosity.

We report herein the preparation of homogeneous silsesquioxane-zinc oxide and silsesquioxane-copper oxide hybrid materials using a non-hydrolytic sol-gel process, though comparable sol-gel materials were reported in the literature to be heterogenous. By varying the synthesis parameters, we developed a range of novel materials. The characteristics of the hybrid materials, including crystallinity, morphology, and surface area, varied significantly with changes in physicochemical parameters such as the drying method, heat treatment, and the types of sol-precursors used. The Si/M molar ratios (M: Zn or Cu) in both aerogels and xerogels were stoichiometric, closely matching those of the initial solutions. The X-ray diffraction study has revealed that the as-synthesized materials were homogeneous at the atomic level as they are predominately amorphous. These results suggest that silica and the other metal exhibit mixed 3D networks with strong bonding interactions. The results salts and the crystalline structures are dispersed at the nano-level into the silica matrix with different morphologies achievable. Heating the metal-containing matrix eliminates organic compounds through oxidation and thermolysis and results in developing mesoporous crystal clusters. These latter are highly dispersed and homogeneously distributed throughout the silica matrix with different morphologies as well. The low degree of crystallinity, the small particle sizes, the high thermal stability, and the high surface area of the annealed samples are attributed to the high dispersion of the metal species obtained.

**Keywords**: Zinc oxide, Copper oxide, Silica, Non-hydrolytic sol-gel process, Aerogels, Xerogels, Nanoporous structures.



**Figure 1**: XRD diffraction patterns and SEM micrographs of as-synthesised silsesquioxanezinc oxide aerogel dried under supercritical conditions, and after being annealed at 400°C.

### Salt-assisted coating of MXene on arbitrary polymers

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#### Abstract:

Two-dimensional carbides and nitrides, known as MXenes, are promising for water-processable coatings due to their excellent electrical, thermal, and optical properties. However, depositing hydrophilic MXene nanosheets onto inert or hydrophobic polymer surfaces presents significant challenges as the interface between the two is vulnerable. Current practices to enhance the interface such as plasma treatment or chemical modification compromise the intrinsic properties of MXene and/or polymer. This research demonstrates a universal salt-assisted assembly method that produces ultra-thin, uniform MXene coatings with exceptional mechanical stability and washability on various polymers, including high-performance polymers for extreme temperatures. The salt in the  $Ti_3C_2Tx$  colloidal suspension reduces surface charges, enabling electrostatically hydrophobized MXene deposition on polymers. A library of salts was used to optimize assembly kinetics and coating morphology. An ultrathin MXene coating can reduce radiation temperature by ~200 °C on a 300 °C PEEK substrate, while the coating on Kevlar fabric provides comfort in extreme conditions, including outer space and polar regions.

## Synergistic Colloidal System from Gellan Gum and Microalgal Extract: Preliminary Insights into Nano Gelation and Structural Properties

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### Abstract:

Soft nanotechnology offers promising avenues for designing eco-friendly colloidal systems. This study investigates the development of bio-based formulations using gellan gum (KF) from Sphingomonas elodea and an aqueous extract (CHLA) of microalgal polysaccharides derived from Chlorella vulgaris. A key finding involved the identification of the glass transition and gelation temperatures of both KF and CHLA in water via differential scanning calorimetry (DSC). Achieving this critical temperature proves essential (1): if the polysaccharide dispersions do not reach it, they fail to form submicron colloidal structures, leading to incomplete or weak gelation upon cooling. The mixture exhibits submicron-scale colloidal water dispersions (ranging from 400 to 450 nm analized by DLS technique) at the gelation point and form stable gel networks upon cooling. Furthermore, the presence of divalent cations significantly influences gellan gum aggregation, favoring a transition from double-helix to triple- or quadruple-helix conformations and increasing the hydration shell structuring (2). Although the exact composition of CHLA, including potential protein content, is still under investigation, preliminary results show that KF/CHLA mixtures gel efficiently even without added divalent cations. SEM analyses confirm the formation of three-dimensional interconnected networks starting from colloidal dispersion (Figure 1), and rheological measurements indicate a clear transition from liquid-like to gel-like behavior. These findings suggest synergistic molecular interactions, possibly involving polysaccharides and residual proteins in the crude extract, leading to unique structural properties. Future work will focus on detailing the chemical constituents of CHLA, elucidating their roles in colloidal gelation, and further evaluating the technological and functional performance of these mixtures as sustainable coating materials. Additionally, preliminary film-formation tests demonstrate promising integrity and cohesive structures, indicating the potential of these colloidal gels as sustainable coatings for food packaging and other applications.

**Keywords**: Gellan Gum, Microalgal Polysaccharides, Colloids, Gel network.



**Figure 1:** SEM image of dehydrated gel structure of KF/CHLA starting from a colloidal dispersion without adding cations

### **References:**

- Sansone, F., Esposito, T., Mencherini, T, Del Prete, F., Cannoniere, A.L., Aquino, R.P. (2023), Exploring microencapsulation potential: Multicomponent spray dried delivery systems for improvement of *Chlorella vulgaris* extract preservation and solubility, *Powder Tech*, 429, 118882
- Tavagnacco, L., Chiessi, E., Severini, L, Franco S, Buratti E, Capocefalo A., Brasili F, Mosca Conte, A., Missori M., Angelini R., Sennato S., Mazzuca C., Zaccarelli E. (2023), Molecular Origin Of The Two-Step Mechanism Of Gellan Aggregation, *Sci. Adv.* 9, eadg4392

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## Synthesis of mesoporous silica nanoparticles in fluoride medium by spray drying

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### Abstract:

Mesoporous silica nanoparticles (MSNs) are usually obtained by conventional sol-gel synthesis techniques, in a process that requires long reaction periods, and goes through many critical steps that condition the morphology, structural and textural properties of the materials. An alternative route for silica nanoparticles manufacturing is the spray drying (SD) technique, which involves particle formation by evaporationinduced hydrolysis and condensation of providing continuous silicates, also production [1]. In this context, we have developed a new SD-based methodology for the preparation of monodispersed MSNs with the MCM-41 hexagonal mesophase by properly adjusting the pH of the synthesis mixture (e.g., pH=8.5), and using NaF as silica mobilizing agent. The formation of MSNs goes through four steps: templating, nucleation, condensation and aging. Templating and nucleation take place very quickly (a few minutes) [2], and it can be assumed that they are happening mostly at the liquid medium before the SD process starts. However, condensation and aging need of a larger period (6-48 hours), specially at neutral pH and room temperature. For spray-dried samples, these steps are accelerated by the fast drying at the hot airflow. The solvent elimination occurs in a few seconds, and the growth of the mesophase depends of an equilibrium between silicate anions condensation and water removal. Fluoride anion is an excellent silica activator even in mild conditions (e.g., neutral pH, room temperature), and it is also able to replace hydroxyl groups from silicate network, reducing the frequency of defects and increasing the stability of the mesoporous structure. Even when the solvent is quickly removed by SD, fluoride is able to catalyze effectively the silicate condensation over CTMA micelles, promoting particle growth and aging in a very short time [3], resulting samples with well-developed MCM-41 structure and textural properties (Figure 1). In addition, optimizing the gas inlet temperature

(T<sub>in</sub>) to 90°C promoted rapid assembly between silicate network building species during the SD process, yielding nanoparticles with good structural and textural properties. In any case, we didn't observe the wet-pocket phenomenon [4], as our nanoparticles were absolutely dried after the SD process, and no significant structural changes were found after template removal. This technique is highly scalable and adaptable to the industrial stage, showing enormous interest in the pharmaceutical development.

**Keywords**: Mesoporous silica nanoparticles; spray drying; fluoride media synthesis; Nano Spray Dryer; drug delivery.



**Figure 1.** Artistic representation of the key steps in MSN preparation by the SD method and classical sol-gel synthesis.

- 1. Vallet-Regí, M., Balas, F., Arcos, D. (2007) Mesoporous materials for drug delivery, Angew. Chem. – Int. Ed. 46, 7548–7558.
- Candela-Noguera, V., Alfonso, M., Amorós, P., Aznar, E., Marcos, M.D., Martínez-Máñez, R. (2024) In-depth study of factors affecting the formation of MCM-41-type mesoporous silica nanoparticles, Microp. Mesop. Mat. 363, 112840.
- Kim, W.J., Yoo, J.C., Hayhurst, D.T. (2000) Synthesis of hydrothermally stable MCM-41 with initial adjustment of pH and direct addition of NaF, Microp. Mesop. Mat. 39, 177–186.
- Waldron, K., Wu, Z., Wu, W.D., Liu, W., Zhao, D., Chen, X.D., Selomulya, C. (2014) Formation of uniform large SBA-15 microspheres via spray drying, J. Mater. Chem. A Mater. 2, 19500–19508.

## DLC film doped with graphene nanoparticles with very low coefficient of friction in ultra high vacuum condition

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### Abstract:

Diamond-like Carbon - DLC Film has been an excellent option, especially as a solid lubricant for many applications in different industrial areas, especially in the space area. In this work we present a study involving measurements of coefficient of friction and wear, with unprecedented results in an ultra-high vacuum environment. DLC films were obtained via Pulsed DC Plasma Enhanced Chemical Vapor Deposition (PECVD), with an important modification that consist of an ion and electron confinement system that allows growing DLC films at very low pressure, 10<sup>-3</sup> Torr, with improved mechanical and trybological properties. For this study, nanoparticles of graphene were added during the growth process in different proportions in relation to the carbon precursors. Acetylene was used as the main carbon precursor and hexane as the auxiliary carbon precursor and also as a carrier of graphene nanoparticles. The dependence of the graphene nanoparticles concentration as a function of the coefficient of friction and wear in an atmospheric environment and in an ultrahigh vacuum environment was studied. As an exceptional result, DLC films with high hardness, excellent adhesion to the titanium substrate were also obtained. Coefficient of friction with values as low as 0.01 were obtained for pressure of 10<sup>-5</sup> Torr. Morphology before and after growth shows that there was no significant change. The identification of the graphene nanoparticles inside of the DLC films with structure was done atomic force microscopy.

**Keywords**: Diamond-like Carbon, Graphene NanoParticles, Coeficient of Friction, Wear, Doping, Solid Lubricant, Space Aplicaton



Figure 1: Diagram of the DLC deposition System

- G. Capote, M. A. Ramírez, P. C. S. da Silva, D. C. Lugo, and V. J. Trava-Airoldi, "Improvement of the properties and the adherence of DLC coatings deposited using a modified pulsed-DC PECVD technique and an additional cathode," *Surf. Coatings Technol.*, vol. 308, pp. 70–79, 2016, doi: 10.1016/j.surfcoat.2016.08.096.
- A.C. Sanches, G. Capote, E.J. Corat, V.J. Trava-Airoldi, Effect of low-pressure deposition on the mechanical and tribological properties of a-C:H films deposited via modified pulsed-DC PECVD with active screen as an additional cathode, Surface &CCoeting Technology, Vol. 445 128716, 2022 doi:10.1016/j.surfcoat.2022.128716

## Nanoscale insight into the functionalization of graphene oxide with porphyrins

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### Abstract:

Graphene oxide (GO) and its reduced counterpart (rGO) have, in several aspects, opposite properties that can be continuously tuned. By analysing the reduction process at the nanoscale, we have recently observed partially reduced flakes consisting of both GO and rGO regions with tuneable sizes.<sup>1</sup> This finding opens the possibility of designing 2D materials that combine the high reactivity of GO with the enhanced conductivity of rGO, paving the way for applications in selective functionalization.

In this study, we investigate the structural, electronic, and optical properties of individual flakes of non-covalent hybrids of GO and rGO and protoporphyrin IX (PPIX) using Kelvin probe force microscopy (KPFM) and optical spectroscopies, including conventional Raman and fluorescence and tip-enhanced Raman scattering (TERS). These techniques provide nanoscale resolution, allowing us to monitor changes within individual flakes with high precision. As shown in Figure 1, TERS maps can spectrally confirm the PPIX coverage of the flakes with a spatial resolution below 35 nm.

Our investigations demonstrate that the reduction degree of GO strongly influences the properties of the resulting hybrid material, affecting the thickness, the homogeneity and the fluorescence spectral features of the PPIX molecules that cover the flakes. Furthermore, fluorescence quenching and light-induced variations in the surface potential prove that charge transfer takes place from PPIX to rGO but not to GO. These findings confirm that PPIX can enhance the optical, electronic, and catalytic properties of rGO, enabling a wide range of applications in energy conversion, biomedical therapy, and pollution mitigation.

**Keywords**: Functional nanomaterials, graphene oxide, porphyrins, monolayer assembly, scanning probe microscopy, surface photovoltage, tip enhanced Raman scattering, photoluminescence.



**Figure 1**: Upper-left map:  $1 \times 1 \mu m^2$  topography of a small rGO flake deposited on an Au substrate (z-scale: 0-3 nm). Upper-right map: integrated TERS intensity ratio of the same flake. Lower spectra: TERS measured on the gold substrate and on the flake showing the Raman peaks of GO (D and G) and of PPIX. One spectrum is shifted for improving clarity.

### **References:**

1. M. Navarro-Rodríguez, V. Camús, et al., Exploring the structure and electronic properties of individual hybrid GO/rGO flakes, Applied Surface Science, 2024, 624, 158611 Nanotech France / NanoMatEn / GAMS 2025 Joint Session I. B: Nanomaterials Modelling, Characterization and Properties

## Determination of size distribution of nanomaterials using Field-Flow Fractionation with different detectors

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### Abstract:

The reduction of materials to the nanoscale introduces unique properties, leading to a growing interest in nanomaterial research. Understanding the relationship between particle size and its functional or application-specific characteristics is crucial for the development of nanotechnology. Nanomaterials find applications in industries such as cosmetics, inks, and food, making accurate size measurement an essential component for their effective use in liquid-phase formulations.

The European Commission defines а nanomaterial as a natural, incidental, or manufactured material containing particles in an unbound state, aggregate, or agglomerate. At least 50% of the particles in the number size distribution must have one or more external dimensions between 1 nm and 100 nm. This definition emphasizes the importance of assessing not only average size but also size distribution, which plays a key role in industrial applications and regulatory compliance for international trade.

Although many sizing techniques exist, selecting the appropriate method remains a challenge. Dynamic light scattering and particle tracking are widelv used to analysis measure nanoparticles in nano- and submicron-scale biocolloidal suspensions. However, the particle sizes obtained can vary depending on the analytical algorithms applied. Electron microscopy provides detailed primary particle information but requires the analysis of a large number of particles, making it a labor-intensive process.

Recent methods, such as field-flow fractionation and flow particle tracking, offer improved accuracy in particle size determination. Hybrid approaches, such as combining field-flow fractionation with electron microscopy, enable simultaneous evaluation of particle size and shape distribution. Each technique has strengths and limitations. This presentation will discuss strategies for selecting the most suitable method based on the specific characteristics and requirements of the nanomaterials being studied.

**Keywords**: size distribution, electron microscope, field-flow fractionation, dynamic

light scattering, static light scattering, laser diffraction, particle tracking analysis, flow particle tracking.

- Kato, H., Nakamura, A. (2023) Novel Colloidal Dispersing Concept in Aqueous Media for Preparation by Wet-Jet Milling Dispersing Method, *Nanomaterials*, 13, 1-15.
- 2. Kato, H., Nakamura, A., Kinugasa, S., Fujimoto, T., (2022) Accurate determination of size distribution of materials in liquid phase, *Synthesiology*, 1, 1-17.
- Kato, H., Nakamura, A., Shimizu, M.,(2022) Effect of surfactant micelle size on the dispersibility of aqueous carbon black particle suspensions prepared by ultrasonication, *Powder Technol.*, 399, 117206.
- 4. Matsuura, Y., Nakamura, A., Kato, H., (2020) Novel Approach for Reliable Determination of the Refractive Index of Particles in the Liquid Phase Using a Hybrid Flow Particle Tracking Method, *Anal. Chem.*, 92, 5994-6002.
- 5. Kato, H., Nakamura, A. (2020) Particle density determination using resonant mass measurement method combined with asymmetrical flow field-flow fractionation method *J. Chromatogr. A.* 1631, 461557.
- 6. Matsuura, Y., Nakamura, A., Kato, H., Determination of an accurate size distribution of nanoparticles using particle tracking analysis corrected for the adverse effect of random Brownian motion, *Phys. Chem. Chem. Phys.*, 20, 17839-17846.
- Matsuura, Y., Nakamura, A., Kato, H. (2018) Determination of Nanoparticle Size Using a Flow Particle-Tracking Method , *Anal. Chem.*, 90, 4182-4187.
- Kato, H., Nakamura, A., Banno H., Shimizu, M. Separation of different-sized silica nanoparticles using asymmetric flow fieldflow fractionation by control of the Debye length of the particles with the addition of electrolyte molecules, *Colloids Surf. A.*, 538, 678-685.

### Theoretical assessment of elastic modulus of carbon nanotubes

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### Abstract:

Nanoscale size of matter has revolutionized the applications of materials. This is because at nanoscale size the material possess new and/or improved properties over its bulk counterpart. The nature of properties depend on the composition, structure and also the size and shape of the material at nanoscale. Apart from new and/or improved properties, nanoscale materials are also nearly defect free and can have magnetic, optical, sensing and actuating properties. Carbon nanotube (CNT) is one such nanoscale material form of bulk carbon. CNTs possess fascinating properties including low density, high strength and modulus, high specific strength and specific modulus, low melting point, high electrical and thermal conductivity, stability at high and low temperatures and a large surface area to volume ratio. Owing to such enhanced properties CNTs find wide range of potential applications as e.g. structural components, or semiconducting conducting wires in nanoelectronic components, probes with chemically functionalized tip in scanningprobe microscopy, high-sensitivity microbalances, gas detectors, hydrogen storage devices by utilizing its large specific area, field-emissiontype displays, electrodes in organic light-emitting diodes, tiny tweezers for nanoscale manipulation and many more.

In order to successfully implement CNTs in potential applications their mechanical properties need to be determined. The elastic modulus or Young's modulus is the most fundamental phenomenological mechanical property of CNTs when deformed under elastic limit. A variety of experimental attempts have been reported in literature to meassure Young's modulus of carbon nanotubes. Estimation of Young's modulus from measurement of thermally induced vibration amplitudes of multiwalled carbon nanotube (MWCNT) cantilever has been reported by Treacy et al. [1]. For MWCNT a range from 0.40 TPa to 4.15 TPa and for SWCNT [2] a range from 0.9 TPa to 1.9 TPa of value of Young's modulus has been reported. Bending experiment on MWCNT cantilever beam acted upon by a lateral force generated by AFM tip predicted Young's modulus of  $1.28 \pm 0.59$  TPa [3]. Poncharal et al. have reported that the

stiffness of MWCNTs decreases quickly when their diameter exceeds about 10nm [4].

Experimental determination of mechanical properties of CNTs is highly cumbersome procedure due to involvement of sophisticated sample preparations and involvement of sophisticated and costly equipments and highly accurate, precise and resolution measurement avoid such costly techniques. To and cumbersome process current work focusses on theoretical assessment of Young's modulus of CNTs. Present paper will demonstrate a two step method of Young's modulud determination viz. initially molecular mechanics approach to predict force deformation behaviour and finally calculation of Young's modulus by conventional strength of materials approach.

**Keywords**: CNT, SWCNT, MWCNT, Young's modulus, molecular mechanics, interaction force, equilibrium separation, chirality.

- Treacy, M. M. J., Ebbesen, T. W., Gibson, J. M. (1996), Exceptionally high Young's modulus observed for individual carbon nanotubes, *Nature*, 381(6584), 678–680.
- Krishnan, A., Dujardin, E., Ebbesen, T.W., Yianilos, P. N., Treacy, M. M. J. (1998), Young's modulus of single-walled nanotubes, *Physical Review B*, 58(20), 14013–14019.
- Wong, E.W., Sheehan, P. E., Lieber, C.M. (1997), Nanobeam mechanics: elasticity, strength, and toughness of nanorods and nanotubes, *Science*, 277 (5334), 1971–1975.
- Poncharal, P., Wang, Z. L., Ugarte, D., Heer, W. A. de (1999), Electrostatic deflections and electromechanical resonances of carbon nanotubes, *Science*, 283 (5407), 1513–1516.

### Growth mechanism and some properties of nanostructured graphene on cubic - SiC / Si (001) wafers

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#### Abstract:

The graphene grown on (001) surface of cubic-SiC/Si wafers usually consist of nanometer-sized domains with a several lattice orientations. In this report we present the in-situ investigation of layer-by-layer graphene growth on such wafers. For measurements we used several modern techniques: scanning tunneling microscopy with atomic resolution, low-energy electron microscopy (LEEM), high-resolution laterallyresolved X-ray photoelectron spectroscopy angle-resolved (micro-XPS), photoelectron spectroscopy (micro-ARPES), and micro lowenergy electron diffraction (micro-LEED). The collected data show the opportunity to control continuously the local thickness of the graphene overlayer on the cubic-SiC(001)/Si wafers in situ during UHV synthesis. Meaningfully, presented data disclose the mechanisms of the surface transformation and layer-by-layer graphene growth on on the (001) surface of the cubic SiC/Si in UHV at elevated temperatures.

**Keywords**: graphene, cubic-SiC, layer-by-layer growth, SPEELEEM, micro-LEED, micro-XPS

**Figure**: Following the continuous evolution of the graphene growth on the surface during the heating process of the  $\beta$ -SiC.



### Graphene as a protecting barrier against metal corrosion

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### Abstract:

Since its isolation in 2004, graphene has proven to be an ideal candidate for several applications, including protecting metals against corrosion. Its tightly packed structure provides complete permeability to gases and salts ions such Cl-, under normal conditions, offering full protection to the substrate from corrosive environments [1] [2]. Moreover, graphene properties allow to preserve the physical properties of the metal substrate, including appearance, electrical and thermal conductivities [1] [2]. In this context, our project focuses on enhancing the corrosion resistance of aluminum and stainless steel using graphene in a marine environment. The graphene was prepared via liquid-phase shear exfoliation, a method that is simple, cost-effective, and environmentally friendly. After subjecting graphene to microscopic and spectroscopic characterization in order to ensure its good qualities, the said nanosheets were deposited on aluminm and steel substrates via spray coating and self-assembly methods. These coatings are characterized then to analyze surface morphology and evaluate their corrosion resistance in a marine environment. These analyses reveal the formation of a high-quality, compact, and continuous thin film with approximately 3 to 7 layers (Figure 1.a). Also, the results showed that graphene effectively protects the surface of aluminum and stainless steel for a good amount of period [3] (Figure 1.b).

**Keywords**: graphene, 2D materials, liquid phase exfoliation, green chemistry, metals, stainless steel, aluminum, corrosion protection, self-assembly, XRD, Raman spectroscopy, SEM, TEM, EIS.



Figure 1: a) Raman spectra, SEM & TEM images of synthesized graphene suspension - c) Nyquist plots of bare and coated aluminum at t = 0 & 30 h along with the chosen circuit equivalent

- Xu, H., Zang, J., Yuan, Y., Tian, P., Wang, Y. (2019) In situ prepration of graphene coating bonded to stainless steel substrate via Cr-C bonding for excellent anticorrosion and wear resistant, *Appl. Surf. Sci.*, 492, 199-208
- Pandey, M., Deshmikh, K., Raman, A., Asok, A., Appukuttan, S., Suman, G. (2024) Prospects of MXene and graphene for energy storage and conversion, *Renew. Sustain Energy Rev.*, 189, 114030
- El Hajj, I., Laïk, B., Gassama, A., Bensifia, M., Dembélé, K., Jama, C., Monnier, J., Léonard, C., Yassar, A., Bouanis, F. (2024) Liquid-phase shear exfoliation of graphite ans its application as corrosion protection coating on aluminum substrate, *Surf. Coat. Technol.* 494, 1314112

## High-performance room-temperature NO<sub>2</sub> gas sensors based on liquid phase exfoliated WS<sub>2</sub> ultra-thin films

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### Abstract:

Transition metal dichalcogenides (TMDs) are a family of semiconducting 2D nanomaterials. Among them, WS<sub>2</sub> stands out due to its theoretically high electron and hole mobilities making a promising material for gas sensing. In this work, we studied the development of a highly sensitive chemiresistive gas sensor based on WS<sub>2</sub> nanosheets for detecting NO<sub>2</sub> at sub-ppm levels under room-temperature. WS<sub>2</sub> nanosheets were synthesized using a highly efficient and eco-friendly liquid phase shear exfoliation (LPSE) method combined with centrifugation, with various parameters optimized to achieve a narrow sheet-size distribution. This method successfully demonstrated the exfoliation of WS2 into few-layer structures (2-3 layers) in an aqueous solution. The interfacial self-assembly method was employed to prepare a highly stacked, continuous WS2 thin film with a thickness of 20-30 nm, making it promising for large-area surface fabrication. The structure and morphology of the WS<sub>2</sub> NSs and ultra-thin films thoroughly characterized were using complementary techniques (UV, DLS, SEM, AFM, TEM, XRD, Raman). The WS<sub>2</sub>-based NO<sub>2</sub> sensor exhibited remarkable sensitivity (23% at 0.5 ppm), fast response (40 s) and recovery times (1800 s), and reliable reversibility, with a theoretical limit of detection (LOD) estimated at 15.8 ppb at room temperature (30°C). This performance can be attributed to the high affinity of WS<sub>2</sub> for NO<sub>2</sub> molecules. The as-prepared sensor demonstrated excellent repeatability, stability and selectivity, confirming its potential for NO<sub>2</sub> sensing applications. Additionally, the effects of humidity and temperature were investigated to assess the sensor's performance under real-world conditions. A mechanism for the NO<sub>2</sub> sensing and humidity detection of WS<sub>2</sub> NSs based sensor has been proposed.

**Keywords**: 2D  $WS_2$  nanosheets; highly compacted ultra-thin films; solution processed method; chemiresistive sensors; NO<sub>2</sub> detection; room temperature.



Figure 1:  $WS_2$ -based  $NO_2$  sensor fabrication using LPSE-SA method,  $WS_2$  nanosheets structure, and sensing performance (sensitivity and repeatability).

- Yan, W., Worsley, M. A., Pham, T., Zettl, A., Carraro, C., & Maboudian, R. (2018). Effects of ambient humidity and temperature on the NO<sub>2</sub> sensing characteristics of WS<sub>2</sub>/graphene aerogel. *Applied Surface Science*, 450, 372-379.
- Kumar, A., Mirzaei, A., Lee, M. H., Ghahremani, Z., Kim, T. U., Kim, J. Y., ... & Kim, H. W. (2024). Strategic review of gas sensing enhancement ways of 2D tungsten disulfide/selenide-based chemiresistive sensors: decoration and composite. *Journal of Materials Chemistry* A, 12(7), 3771-3806.

## Defect control of graphene using ion beam irradiation and its application to gas sensing.

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#### Abstract:

Defects in graphene significantly influence its properties and potential industrial applications. The precise control of these defects is therefore crucial. Ion beam irradiation emerges as a vital tool for fine-tuning the defect density in graphene. In this presentation, we explore the evolution of defect density under varying ion beam irradiation conditions using Raman spectroscopy data, and introduce a universal law that correlates defect density in graphene with the ratio I(D)/I(G). Here, I(D) and I(G) correspond to the intensities of the defect peak near 1350 cm<sup>-1</sup> and the G peak near 1580 cm<sup>-1</sup> in Raman spectra, respectively, illustrated in Figure 1. Additionally, by integrating electrodes on graphene, we examine resistance changes when exposed to gases like acetone, CO, NH3, and NO2. Of particular interest, graphene with an optimal defect concentration exhibits greater resistance changes compared to pristine graphene, reflecting enhanced sensitivity. Although graphene gas sensors can detect various gases, this talk specifically addresses acetone sensing, as demonstrated in Figure 2. Moreover, Kr ion irradiation is found to improve sensor sensitivity, with resistance changes being highly dependent on the irradiation conditions. We will discuss how sensitivity varies with Kr beam parameters and acetone concentration.

**Keywords**: Graphen, Defect Engineering, Ion beam irradiation, Gas Sensors, Raman Spectroscopy, 2-D material application.



Figure 1: The defect yields (I(D)/I(G)) under different ion beam irradiation conditions are

collapsed onto the same curve,  $C(1-exp(-\alpha Ld))$ 

where  $\alpha$ , *L*, and *d* are fitting coefficient, nuclear LET (linear energy transfer), and dose, respectively.





**Figure 2**: Kr irradiation at 80 keV with a dose of  $1 \times 10^{13}$ #/cm<sup>2</sup> shows the largest resitance change for a 1% acetone flow.

- Yeo, S., Han, J., Bae, S., Lee, D. (2018), Coherenc in defect evolution data for the ion beam irradiated graphene, *Scientivic Report*. 8, 13973
- Yeo, S., Lee, C. Y., Kim, D.-S., Hwang, Y. S., Park, J. K., Jung M.-H., Cho, W.-J. Lee, J. S., Kim, C. (2019), Sensing response enhancement of graphene gas sensors by ion beam bombardment, *Thin Solid Films.*, 677, 73-76.

## First steps with DFT for plasmon mapping in modified graphene for sensor development

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### Abstract:

Plasmons for detecting molecules should be accompanied by an understanding of the interactions between surface and molecule. Here, we used density functional theory by Quantum Espresso software to reach the mentioned goal.

With this tool, we are looking to create a map to develop more accurate sensors based on graphene. We explored the variations in the electron energy loss spectroscopy (EELS) and the constraint loss of graphene-modified -it means with vacancies and doped with fluor, nitrogen, and oxygen. We studied seven percentages for each graphene-modified layer, from 0.78% to 12.5%. Additionally, we present findings on graphene oxide (GO) doped with 8% oxygen and reduced graphene oxide (rGO) at the percentages specified in Shilpent's datasheet.

Our results show that graphene doped with as little as 2% oxygen exhibits out-of-plane plasmons in the green region of the spectrum. Additionally, graphene containing more than 5% oxygen shifts the plasmon peak into the violet region. Graphene with less than 6% nitrogen demonstrates in-plane plasmon activity in the infrared region. Doping graphene with fluorine between 3% and 5% results in in-plane plasmons in the blue region. Finally, graphene with more than 5% vacancies presents multiple peaks in the visible region.

This research is significant as it helps us identify which type of graphene is most effective for use in different spectral regions. Understanding the behavior of each layer will further aid in developing advanced sensors. **Keywords**: Graphene, plasmons, optical sensors, ab-initio calculations.

### Nanostructured In<sub>2</sub>O<sub>3</sub> Gas Sensors for Ultra-Sensitive H<sub>2</sub>S Detection at Trace Levels

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### Abstract:

In recent years, there has been a growing focus on improving gas sensor technology, which plays a vital role in detecting harmful gases in the environment [1,2]. Emissions from industries, automobiles, and other sources release pollutants such as CO, NO<sub>2</sub>, H<sub>2</sub>S, and NH<sub>3</sub> into the atmosphere, which negatively affect human health.[3,4] These pollutants contribute to significant health risks and environmental challenges. Among these, gases like H<sub>2</sub>S are particularly hazardous due to their toxicity, even at low concentrations, posing serious threats to human well-being.

Achieving high selectivity and sensitivity for specific analytes at trace levels remains a significant challenge for chemiresistive gas sensors. In this study, nanostructured indium oxide (In<sub>2</sub>O<sub>3</sub>) gas sensors were fabricated using the spin coating technique to detect hydrogen sulfide (H<sub>2</sub>S) gas at low concentrations. The impact of annealing temperature on the gas sensing performance of the nanostructured sensors was systematically examined. The sensor annealed at 350°C exhibited remarkable performance, with a rapid response time of  $(17 \pm$ 1) seconds for 4 ppm H<sub>2</sub>S gas at an optimal operating temperature of 250°C. Additionally, it showed excellent sensing responses of (36.52  $\pm$ 2.02) % for 0.5 ppm and  $(97.89 \pm 0.08)$  % for 4 ppm H<sub>2</sub>S gas. This exceptional performance is attributed to the structural defects, voids, and oxygen vacancies enhances gas adsorption and reactivity. The finding here demonstrates In<sub>2</sub>O<sub>3</sub> nanostructured gas sensors are highly effective for the reliable detection and monitoring of H<sub>2</sub>S gas in real-world applications.

The remarkable sensing performance is attributed to the presence of structural defects, voids and oxygen vacancies, which enhance gas adsorption and reactivity. These findings demonstrate that In2O3 nanostructured gas sensors are highly effective for the reliable detection and monitoring of H2S gas in practical applications.

**Keywords:** In2O3, Nanostructure, H2S gas, Sensing mechanism, gas sensors, oxygen vacancies.



**Figure 1:** In<sub>2</sub>O<sub>3</sub> Sensor Response at different concentrations of H2S gas

- Li Z, Li H, Wu Z, Wang M, Luo J, Torun H, Hu P, Yang C, Grundmann M, Liu X, Fu Y. (2019) Advances in designs and mechanisms of semiconducting metal oxide nanostructures for high-precision gas sensors operated at room temperature. Mater Horiz., 6, 470–506.
- Kiani M, Rehman MU, Tian X, Yakobson B. (2022) Two-Dimensional Nanomaterials for the Development of Efficient Gas Sensors: Recent Advances, Challenges, and Future Perspectives. Adv Mater Technol.,7, 202101252.
- Badadhe SS, Mulla IS., (2011) Effect of aluminium doping on structural and gas sensing properties of zinc oxide thin films deposited by spray pyrolysis. *Sens. Actuators B Chem.* 156, 943–8.
- Z. Jin, Y. Mou, J. Zhao, C. Chen, H. Zhou, N. Xiang, F. Wang, Z. Wang, J. Liu and L. Wu, (2024), H<sub>2</sub>S gas sensing enhancement of Au-decorated SnO<sub>2</sub> nanospheres synthesized using hydrothermal and microwave methods *Sens. Actuators B Chem*, 401, 135026.

## Nanomaterials for Extreme Environments: From Heteronanotubes to High-Performance Fibres

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### Abstract:

A systemic approach to designing and manufacturing advanced materials such as carbon- and ceramic-based nanomaterials, their hybrids, and advanced polymer design is critical for these materials to perform reliably in extreme environments that are typically found in the aerospace, defence, and energy sectors.

Control over the thermal, mechanical, and chemical mechanical properties is achieved through the careful design and development of state-of-the-art manufacturing of nanoscale heteronanotubes (e.g., MWCNT@BNNTs),[1,2] macroscale ceramic fibre assemblies (e.g. BN, SiO2/ZrO2, SiO2/Al2O3, SiO2/TiO2)[3–5] and polymer fibres[6,7], integrating structural resilience, thermal stability, and multifunctionality.

For example, designing scalable synthesis, we demonstrate coaxial CNT@BNNT structures combining the conductivity of carbon nanotubes with the thermal and chemical robustness of boron nitride. These heteronanotubes, fabricated into buckypapers, show enhanced thermal conductivity and offer new routes for multifunctional composites

Complementing this, we develop a singleprecursor system electrospinning route to fabricate pure h-BN fibres with high B–N purity and temperature stability above  $1300 \,^{\circ}$ C. In parallel, we engineer sol-gel systems to modulate the fibre assemblies 2D to 3D morphology, achieving ultralow density and low thermal conductivity (~21.6 mW/m·K), produced through an electrospinning method.[8] These structures enable directional heat flow and can be made hydrophobic for use in corrosive or humid environments.

Ultrathin electrospun poly(3-hexylthiophene) (P3HT) nanofibres were developed through the incorporation of plasmonic nanoparticles, which modulate solution viscosity and eliminate the need for excessive solvents. This approach led to fibres that demonstrate a 58% performance enhancement in organic photovoltaics compared to thin films, attributed to a combination of plasmonic effects and enhanced polymer chain alignment induced by electrospinning.

Together, this research delivers integrated materials from nanostructured heteronanotubes to self-supporting ceramic macrostructures, tailored for lightweight protection, thermal management, organic photovoltaics applications and durable performance in extreme conditions.

- 1. Maciejewska, O. Kolosov, N. Grobert, ACS Appl. Nano Mater. 2023, 6, 15374.
- 2. R. S. Jones, B. Maciejewska, N. Grobert, Nanoscale Adv. 2020, 2, 4996.
- S. Dong, G. T. Tebbutt, R. Millar, N. Grobert, B. M. Maciejewska, Mater. Des. 2023, 234, 112318.
- 4. S. Dong, B. M. Maciejewska, R. Millar, N. Grobert, ACS Nano 2023, 17, 6800.
- G. N. Dong Shiling, Maciejewska Barbara, Schofield Ryan, Hawkins Nicholas, Siviour Clive, ACS Nano 2024, nn-2023-12.
- R. M. Schofield, B. M. Maciejewska, S. Dong, G. T. Tebbutt, D. McGurty, R. S. Bonilla, H. E. Assender, N. Grobert, Adv. Compos. Hybrid Mater. 2023, 6, 1.
- R. M. Schofield, B. M. Maciejewska, K. A. Elmestekawy, J. M. Woolley, G. T. Tebbutt, M. Danaie, C. S. Allen, L. M. Herz, H. E. Assender, N. Grobert, R. M. Schofield, B. M. Maciejewska, G. T. Tebbutt, C. S. Allen, H. E. Assender, N. Grobert, Small 2025, 21, 2409269.
- S. Dong, B. M. Maciejewska, M. Lißner, D. Thomson, D. Townsend, R. Millar, N. Petrinic, N. Grobert, ACS Nano 2023, 17, 6800.

### FTIR study of Carbonated MgO under Thermal and Plasma treatments

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#### Abstract:

MgO adsorbs atmospheric water and CO<sub>2</sub>, forming surface carbonate species (it becomes carbonated <sup>(1)</sup>). In this work, we present the evolution of FTIR spectra of commercial MgO (Sigma-Aldrich) during thermal treatment up to 350 °C in comparison to plasma treatment with Ar or O<sub>2</sub> (Glow Discharge).

BET specific surface was 189 m<sup>2</sup>/g. TGA (Figure 1) showed the presence of 5% MgCO<sub>3</sub> and 6% Mg(OH)<sub>2</sub> in addition to 10% water (adsorbed or in hydrated MgCO<sub>3</sub> structure).

FTIR spectra were collected at 700-6000 cm<sup>-1</sup> on self-supporting MgO wafers using a Bruker Vertex 80v FTIR spectrometer equipped with a MCT detector and a vacuum cell with KBr windows. The initial spectrum (Figure 2 and 3) displayed the typical carbonate bands including fundamental vibration modes (v3 around 1450 cm<sup>-1</sup>, v1 at 1100 cm<sup>-1</sup>, and v2 at 870 cm<sup>-1</sup>) in addition to combination bands. Moreover, the spectrum displayed a wide peak due to adsorbed water and H-bonding around 3400 cm<sup>-1</sup>. In addition, the peak at 3690 cm<sup>-1</sup> corresponds to -OH groups which is consistent with the presence of Mg(OH)<sub>2</sub>. It is noteworthy that the high intensity peak around 1450 cm<sup>-1</sup> is a composite peak of carbonate v3, water and -OH groups. Upon heating (2-5 hours at each temperature till stability, Figure 2), physisorbed water (5170 and 1640 cm<sup>-1</sup>) was removed at 50°C, and chemisorbed water gradually desorbed till 150-200°C. At 250°C, the carbonate decomposed, and hydration water was liberated. At  $\geq$ 300°C, only the -OH peaks persisted. There are probably several types of -OH groups, given the several observed residual peaks.

Interestingly, plasma treatment (Figure 3) under Ar for only 5 min achieved the same as 2-5 hours heating at 150-200°C. Furthermore, replacing Ar by O<sub>2</sub> had the same effect as 300-350°C heating. Longer exposure to O<sub>2</sub>(10 min) further lead to an equivalent effect as heating at (T > 350 °C).

These results show the remarkable ability of Plasma treatment to eliminate strongly bound adsorbates at RT, which could be beneficial for energy-efficient recycling of gas-capture materials.

**Keywords:** MgO, FTIR, Plasma, Glow Discharge, TGA, Carbonate, Adsorption.



**Figure 1**: TGA profile of MgO up to 800 °C using a 1°C/min heating ramp.



**Figure 2**: Evolution of FTIR spectra of carbonated MgO during heating from RT to 350°C under vacuum. The empty yellow circles correspond to carbonate combination bands.



Figure 3: FTIR spectra of carbonated MgO before and after treatment with Plasma Glow-Discharge under Ar or  $O_2$  flow.

#### **References:**

 Ni, J., Meunier, F. C., Robles-Manuel, S., Barrault, J., Valange, S. (2011) Characterization of surface acidity of carbonated materials by IR-sensitive molecular probes: Advantages of using tertbutyl cyanide, J. Phys. Chem. C, 115, 24931–24936.

## Zinc Oxide Aerogel for Water Remediation

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### Abstract:

Environmental pollution from colored effluents poses a significant global challenge [1]. Whereas adsorption is the most common method for treating dye-contaminated water, zinc oxide nanomaterials are promising adsorbents for the removal of Methylene Blue (MB) [2]. In this work, zinc oxide aerogel was evaluated as an efficient adsorbent for removing MB and CR from aqueous solutions using batch processes. Various operating parameters, including adsorbent dosage (2.5–20 mg), contact time (3– 120 min), and initial dye concentration (20-250 systematically studied. were The ppm), adsorption process was assumed to be independent of pH and temperature within the experimental range. Adsorption kinetics and isotherms were analyzed using both linear and nonlinear regression methods. Under optimal conditions (adsorbent dosage: 7.5 mg, contact time: 50 min, dye concentration: 60 ppm), the maximum adsorption capacity (Q<sub>m</sub>) for MB reached 101.5 mg/g, achieving 85% dye removal. The ZnO aerogels were synthesized through a cost-effective one-pot sol-gel route using zinc nitrate as the zinc precursor and tetramethyl orthosilicate (TMOS) as the silica precursor, with epoxide as the gelation agent. Followed by CO<sub>2</sub> supercritical drying. Characterization techniques, including Scanning Electron Microscopy (SEM), Brunauer-Emmett-Teller (BET) analysis, and Thermogravimetric Analysis (TGA), confirmed the formation of aerogels with a high surface area of 210 m<sup>2</sup>/g, a wide pore volume of 1 cm<sup>3</sup>/g, and excellent thermal stability up to 800°C. The aerogel possesses an extremely low density of 0.16 g/cm<sup>3</sup>, which has been shown to aid in creating a stable suspension in solution. This study highlights the potential of ZnO aerogel synthesized via a one-pot sol-gel process at ambient temperature as efficient adsorbents for wastewater dye remediation, owing to their high surface area, thermal stability, and cost-effective preparation.

**Keywords**: Zinc oxide; Silica; Non-hydrolytic sol-gel process; Aerogels; Xerogels; Nanoporous structures.



**Figure 1**: Figure illustrating the fundamental adsorption process of MB on the ZnO aerogel surface, highlighting the hierarchical porosity of the aerogel structure and the proposed adsorption mechanism.

#### **References:**

[1] O Tünay, I Kabdasli, G Eremektar, D Orhon (1996) Water Science and Technology 34: 9. Doi:https://doi.org/10.1016/S0273-1223(96)00815-3

[2] F Akhter, M Pinjaro, J Ahmed, et al. (2024) Biomass Conversion and Biorefinery: 1. Doi:10.1007/s13399-024-05469-6
## Poly(2,6-dimethyl-1,4-phenylene)oxide (PPO) nanoporous crystalline films for water remediation

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#### Abstract:

Industrial, agricultural and domestic wastewaters are significantly changing the quality of natural reservoirs: it is essential to continually develop innovative and effective strategies for pollutant removal [1].

Among different strategies involved in water remediation, adsorbtion is one of the most used process because it is easy-to-perform, costeffective and does not involves chemicals or the presence of intermediates of reactions: for these reasons, it is essential to introduce new sorbents materials, and using nanoporous crystalline (NC) polymers, is a very promising way to enhance the adsorbtion process. In particular syndiotactic polystyrene (s-PS) and poly(2,6-dimethyl-1,4phenylene)oxide (PPO) have already been studied [2,3], but among them PPO shows unique properties such as higher thermal and chemical stability, and fast kinetics uptake of pollutant from dilute aqueous solutions, when it is used in its NC form [4].

In this study, uptake of pollutants (i.e.: perchloroethylene, atrazine, phenols) from dilute aqueous solution are studied by using PPO in its amorphous form and its NC form, in order to higlight the different sorption capacity, uptake and kinetics between the amorphous phase, and the nanoporous crystalline phase. Adsorbtion kinetics have been studied for the amorphous and NC systems, showing that faster kinetics and higher pollutant amount sorbed are reached when the NC phase is involved in the sorbtion process.

**Keywords**: porosity, nanoporous crystalline polymers, water remediation, wastewater, kinetics

#### **References:**

- 1. Tundwal, A., Kumar, H., Binoj, B. J., Sharma, R. et al. (2024) Conducting polymers and carbon nanotubes in the field of environmental remediation: sustainable developments, *Coord. Chem. Rev.*, 500, 21533.
- Guerra, G., Daniel, C., Rizzo P., Tarallo, O. (2012) Advanced materials based on

polymer cocrystalline forms, J. Polym. Sci., Part B: polym. Phys., 5, 305-322.

- Rizzo, P., Gallo, C., Vitale, V., Tarallo, O., Guerra, G. (2019) Nanoporous-crystalline films of PPO with parallel and perpendicular polymer chain orientations, *Polymer*, 167, 193-201.
- 4. Cozzolino, A., Nagendra, B., Rizzo, P., Daniel. C., Guerra, G. (2021) Fast uptake of organic pollutants from dilute aqueous solutions by nanoporous-crystalline PPO films with c-perpendicular orientation, *Eur. Polym. J.*, 161, 110864.

#### Acknowledgements:

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## Enhanced water desalination via Direct Contact Membrane Distillation using Polyacrylonitrile-derived carbon nanofiber membranes

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#### Abstract:

Water scarcity remains a critical global challenge, intensifying the demand for innovative desalination technologies that are both efficient and sustainable. As the availability of freshwater resources continues to decline due to population growth, climate change, and industrial expansion, there is an urgent need for solutions that can meet these increasing demands.

Direct Contact Membrane Distillation (DCMD) has emerged as a promising approach, combining simplicity, versatility, and energy efficiency. By utilising thermal gradients, DCMD facilitates the effective separation of water vapor from saline solutions, achieving high salt rejection rates while operating under relatively low-temperature conditions (60-80°C). This positions DCMD as a viable and adaptable option for addressing the growing water crisis.

In this study, we investigate the performance of membranes fabricated from Polvacrylonitrile nanofibers, synthesized via (PAN) the electrospinning technique. The PAN nanofibers undergo a pre-treatment process involving calcination, where heating induces the transformation of the fibers into carbon nanofibers. This process enhances their structural, thermal, and mechanical properties, which are tailored to optimize the membranes' The performance in water desalination. distinctive structure of PAN nanofibers, characterized by high porosity (above 80%) and mechanical stability, enables superior performance in DCMD systems, as confirmed through various characterization methods including Scanning Electron Microscopy (SEM) and Porosimetry. Additionally, a customdesigned DCMD pilot system (Figure 1) was developed and employed in our experiments. The system was operated with feed solutions containing 3% NaCl, and the experimental evaluations demonstrated that the calcined PAN membranes exhibited high salt rejection.

These results highlight the potential of calcined PAN nanofiber membranes for exceptional water vapor flux and high salt rejection, validating their suitability for efficient desalination applications.



This work lays the foundation for advancing next-generation membrane materials, setting the stage for improved efficiency and accessibility in desalination processes.

**Keywords**: Desalination, DCMD, Electrospinning, PAN, Salt rejection.

**Figure 1**: Desalination using PAN membrane in a DCMD pilot system.

- Tauk, M., Bechelany, M., Sistat, P., Habchi, R., Cretin, M., & Zaviska, F. (2024). Ionselectivity advancements in capacitive deionization: a comprehensive review. Desalination, 572, 117146.
- Subrahmanya, T. M., Austria, H. F. M., Chen, Y. Y., Setiawan, O., Widakdo, J., Kurkuri, M. D., ... & Lai, J. Y. (2024). Selfsurface heating membrane distillation for sustainable production of freshwater: A state of the art overview. Progress in Materials Science, 101309.

## Nanotech France/ NanoMatEn/ GAMS 2025 Joint Plenary Session II

# A cryogenic energy efficient memory cell for quantum and neuromorphic computing

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#### Abstract:

A substantial demand for high-performance computing systems with low power consumption is created by the exponential growth in data processing. This demand is a significant challenge classical computers based on to Silicon complementary metal-oxide-semiconductor (CMOS) technology. Potential solutions include cryogenic computing as well as novel computing paradigms like neuromorphic<sup>1,2</sup> (NC) and quantum computing<sup>3</sup> (QC). In QC, extremely low cryogenic temperatures (<<1 K) preserve quantum coherence, however cryogenic temperatures are also beneficial for classical von Neumann circuits based on CMOS technology: The reduction of supply voltage at cryogenic temperatures offers significant power savings beyond requirements for cooling. Here, reduced subthreshold swing (SS) and increased mobility lead to increased energy efficiency and high-performance operations. Adding NC architectures at cryogenic computing will further substantially decrease the power demands. Moreover, machine learning can play a pivotal role in tuning semiconductor spin qubits, in realizing error correction decoder and analyzing qubit information. For these applications circuits should operate at 1K - 4.2 K. These trends open up prospects for universal cryogenic computing (UCC) combining benefits of von Neumann, NC and QC information processors for large-scale data processing. The realization requires also a high density low power memory, however, no clear path exists to date.

We report a new cryogenic capacitorless RAM (C<sup>2</sup>RAM) cell based on a fully depleted Silicon on Oxide metal-oxide-semiconductor field-effect transistor, featuring an ultra-thin Si body and an ultra-thin buried oxide (BOX). The proposed C<sup>2</sup>RAM structure and it working principle is depicted in Figure 1. The energy efficient  $C^2RAM$ approach is fully scalable and suppresses short channel effects. It can be extended to multi-state capability. C<sup>2</sup>RAM does not store charges in the channel layer, instead locates them at the Si substrate-BOX interface, separating them from channel carriers and source/drain junctions. This significantly improves the retention time, allowing for non-volatile memories

**Keywords**: Cryogenic CMOS, capacitorless memory, low power computing



Figure 1:  $C^2RAM$  structure and working principles. **a**. Device operating at a low V<sub>D</sub>. **b**. Energy band diagram at substrate surface. **c**. I<sub>D</sub> - V<sub>G</sub> characteristics showing "0" state (high threshold voltage V<sub>th</sub>). **d**. Charge distribution in the substrate for state "1" (negative drain voltage V<sub>D</sub>). **e**. Energy band diagram at substrate surface showing the impact ionization due to V<sub>D</sub>. **f**. I<sub>D</sub> -V<sub>G</sub> characteristics showing "1" state (small V<sub>th</sub>). Memory window defined by the voltage difference of "0" and "1" state. **g**. Charge distribution during erase. h. Energy band diagram at substrate surface showing erase process. **i**. I<sub>D</sub>-V<sub>G</sub> characteristics showing "0" state after erase.

- G. Migliato Marega, Y. Zhao, A. Avsar, Z. Wang, M. Tripathi, A. Radenovic, A. Kis, Logic-in-memory based on an atomically thin semiconductor. Nature 587, 72–77 (2020).
- F. Xi, A. Grenmyr, J. Zhang, Y. Han, J. H. Bae, D. Grützmacher, Q. T. Zhao, Heterosynaptic Plasticity and Neuromorphic Boolean Logic Enabled by Ferroelectric Polarization Modulated Schottky Diodes. Adv. Electron. Mater. 9, 1–12 (2023)
- 3. T. D. Ladd, F. Jelezko, R. Laflamme, Y. Nakamura, C. Monroe, J. L. O'Brien, Quantum computers. Nature 464, 45–53 (2010)

Biological mechanisms of actions of nanomaterial-induced respiratory toxicity Ulla Vogel<sup>1</sup> <sup>1</sup>National Research Centre for the Working Environment, Copenhagen, Denmark

#### Abstract:

Nano-sized particles are more hazardous to inhale than larger particles with the same chemical composition. This is especially true for insoluble particles. In addition, shape and solubility are important predictors of toxicity.

Inhalation of particles is linked to increased risk of cancer, cardiovascular disease, fibrosis and COPD and Adverse Outcome Pathways to describe the causal relationships have been proposed.

Following inhalation, alveolar deposition is determined by particle size distribution. The alveolar deposition leads to low clearance rates, resulting in high lung burden. High- aspect-ratio nanomaterials have very low clearance rates, similar to asbestos.

Particle presence in the lung induces inflammation and acute phase response, which are proportional to the deposited surface area. Acute phase response is a risk factor for cardiovascular disease, and inflammation is linked to fibrosis, cancer and COPD. Other putative mechanisms-of-action for carcinogenicity include frustrated phagocytosis of high-aspect-nanomaterials, and particleinduced generation of reactive oxygen species and oxidative stress.

Examples of health-based occupational exposure limits will be presented for the process-generated nanoparticle diesel engine exhaust, for insoluble nanoparticles such as carbon black and titanium dioxide, for the asbestos-like carbon nanotubes and for the soluble ZnO. In addition, the pathway to societal impact of the research is described. **Keywords**: nanoparticle, ultrafine particle, cancer, cardiovascular disease, fibrosis, risk assessment, occupational exposure limit

### Multifunctional carbon dots for imaging and therapy

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#### Abstract:

Carbon dots have been identified more than 20 years ago and with time they started to attract a lot of attention, as they are considered promising nanomaterials for future clinical translation.<sup>1</sup> Carbon dots combine numerous characteristics including high photostability, low cytotoxicity, and superior biocompatibility. One important aspect related to the synthesis of carbon dots is the assessment of their purity (Figure 1).<sup>1</sup> We applied several methods to prepare carbon dots, using small precursors or polymers.<sup>2,3</sup> We have conceived and synthesised multifunctional carbon dots with deep-red emission properties through their controlled chemical modification using folic acid ligand. These conjugates, endowed of a high colloidal stability and an enhanced luminescence, are suitable for targeted intracellular production of reactive oxygen species by laser irradiation leading to efficient cancer cell death.<sup>3</sup> In addition, we have modified the carbon dots with a chelating agent for gadolinium.<sup>4</sup> These dots showed a better magnetic resonance relaxivity than commercial magnetic resonance imaging (MRI) agents, clinical resulting potential tools 25 MRI/fluorescence dually functional imaging probes. Aimed to phototherapy applications, multifunctional carbon dots were modified with folic acid and chlorin e6. The resulting dots were endowed with near-infrared (NIR) fluorescence photosensitizing enhanced NIR emission. properties, and high photothermal activity. They efficiently targeted and penetrated cancer cells, leading to cell killing under NIR laser irradiation. They also displaied a long blood circulation time in mice.<sup>5</sup>

**Keywords**: Carbon materials, graphene, biomedical applications, cancer therapy, biodegradation, drug carrier, phototherapy, blood circulation.



Figure 1: Carbon dots' (CDs) purification methods: diverse purification techniques, including centrifugation, filtration, dialysis, column chromatography, and electrophoresis, should be systematically applied to assess carbon dot purity.

- 1. Hu, Y., Seivert, O., Tang, Y., Karahan, E., Bianco, A. (2024) Carbon Dot Synthesis and Purification: Trends, Challenges and Recommendations. *Angew. Chem. Int. Ed.*, 63, e202412341.
- 2. Hu, Y., Bianco A. (2025) Unraveling the synthesis-structure-property relationship in aromatic amino acids-derived carbon dots. *Carbon*, 235, 120073.
- Ji, D.-K., Reina, G., Guo, S., Eredia, M., Samorì, P., Ménard-Moyon, C., Bianco A. (2020) Controlled Functionalization of Redemissive Carbon Nanodots for Targeted Intracellular Production of Reactive Oxygen Species. *Nanoscale Hor.*, 5, 1240-1249.
- Ji, D.-K., Reina, G., Liang, H., Zhang, D., Ballesteros, B., Ménard-Moyon, C., Li, J., Bianco, A. (2021)Functional carbon nanodots for T1-weighted magnetic resonance imaging. ACS Appl. Nano Mate., 4, 1467-1477.
- Ji, D.-K., Dali, H., Guo, S., Malaganahally, S., Vollaire, J., Josserand, V., Dumortier, H., Ménard-Moyon, C., Bianco A. (2022) Multifunctional Carbon Nanodots: Enhanced NIR Photosensitizing, Photothermal Activity and Body Clearance. *Small Sci.*, 2, 2100082.1

## Automated Atomic Scale Data Analysis and Modelling for (Scanning) Transmission Electron Microscopy

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#### Abstract:

The process of discovering and refining new materials, as well as enhancing existing ones for a variety of uses, including quantum applications, is a complex and multifaceted endeavor. This involves identifying needs, reviewing existing literature, proposing materials, engineering devices, characterizing materials, and testing applications.

In this digital age and with quantum supremacy in the horizon, semiconductor heterostructures within a chip have become indispensable and ubiquitous, propelling significant industrial value chains. They facilitate progress in both emerging sectors like quantum applications and established ones. For that, the trend of miniaturization, which is now reaching nanoscale dimensions and nearing the atomic limit, is a key driver of progress which demands special characterization needs. [1,2] To answer these needs, we present different solutions relying on AI-enhanced analytical frameworks based on ML/DL, which automates TEM data analysis,[3] aimed at the comprehensive characterization of materials and device structures, with a particular focus on materials for energy and environmental applications, as well as quantum devices and their related heterostructures.

The characterization that must answer these demands is Transmission Electron Microscopy (TEM), as the most optimal way to access structural information at the atomic level. We propose a workflow capable of processing both parallel illumination TEM and Scanning TEM (STEM) data, although it is specially designed for the latter. In addition, it can extract compositional information from Electron Energy Loss Spectroscopy (EELS), which is used to make the characterization an exhaustive and complete process. Importantly, the workflow we suggest combines traditional algorithmic, with unsupervised and supervised machine learning algorithms. This way, we ensure that modelbased computing and artificial intelligence work hand by hand to provide the comprehensive and material-independent solution we seek for. [3]

Our pioneering workflow autonomously determines material composition, crystallographic phase, and spatial orientation across various regions of (S)TEM-based images or image datasets through detailed model comparison. It is completed with automated strain analysis, enabling a comprehensive characterization of the device's structural properties. Eventually, we incorporate the extracted knowledge to automate the creation of models that could facilitate theoretical simulations and would provide vital physical and chemical insights necessary for understanding device's performance in practical the applications. [3]

We have proved it with SiGe quantum well heterostructures that demonstrated outstanding quantum performance for spin qubits generation. [1,2] However, we demonstrate how it works for different material configuration and not only does it answer the pressing automation needs but unlocks getting physical models and simulations of complex devices with unprecedented accuracy.[4]



**Figure 1**: Global workflow of our methodology applied to the study of Ge/Si devices.

- 1. Jirovec, D. et al. Nature Materials, (2021)
- 2. Paquelet, B. et al Nat. Commun. 14, 1385 (2023).
- 3. Botifoll M., Pinto-Huguet I., et. al, Nanoscale Horizons, 7, 1427 (2022)
- 4. Botifoll M., Pinto-Huguet I., et. al, submitted (2025)

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

## Functionalized Nanodiamond Fluids in Transformers Thermal Management – A CFD Modeling Study

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#### Abstract:

Pole-mounted transformers are widely used in the United States and various other regions of the world, but their thermal management is severely limited. The thermal management primarily relies on the mineral oil contained within the transformer walls and surrounding the core. The transformer's core generates heat during operation, and the mineral oil facilitates heat dissipation through heat transfer mechanisms. The mineral oil currently in use globally is a which resists dielectric oil. electrical conductivity. This oil is predominantly utilized because it is inexpensive to produce and acquire, while also possessing high thermal properties. Discovering a method to further enhance these thermal properties could not only boost the efficiency and longevity of the transformer but might also increase its output. Employing nanodiamond enhanced mineral oil presents a potential solution to improve the thermal properties of the existing system, which is both affordable and causes minimal change to the current setup and functionality of the transformers. This enhancement could be achieved by incorporating a by-product from other processes into the dielectric mineral oil currently employed in pole-mounted transformers. This change would impact not just newly manufactured transformers but also those already in operation, as the sole modification would be the oil inside the transformer's walls. Previous research by the author indicates that introducing nanodiamond particles into dielectric mineral oil alters its physical and thermal characteristics. Depending on the concentration of functionalized nanodiamond particles added to the oil, both thermal conductivity and specific heat can increase. Considering this and previous findings, this paper will explore the possible and anticipated changes using CFD modeling of the transformer for both the conventional mineral oil scenario and the functionalized nanodiamond enhanced mineral oil scenario. These scenarios will examine the temperature distribution throughout the transformer as a whole. Additionally, these scenarios will assess the overall heat transfer capabilities of both types of oil over time and compare the results from each

mineral oil to evaluate the overall improvements and effectiveness of utilizing functionalized nanodiamond enhanced mineral oil.

**Keywords**: nanodiamond, transformers, thermal management, CFD modeling

## Materials and Surface Engineering for Outdoor Electrical Insulation

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#### Abstract:

Instrument transformers, embedded poles, electric cables, and sensors are integral components of outdoor electrical distribution systems, requiring exceptional insulation properties to ensure reliability and longevity, while at the same time being able to withstand harsh weather environments and fire threats that could potentially disrupt their operation. With this work we would like to address the critical challenges and advancements in the field of electrical insulation, emphasizing the importance of robust materials and innovative surface engineering techniques.

For electrical insulation, typically polymeric materials are used which need to satisfy key properties such as high dielectric strength and minimal leakage currents. When used outdoors, several additional requirements come into consideration, such as resistance to UV exposure, moisture resistance (hydrophobicity), thermal stability, mechanical strength, etc. To develop appropriate materials for this application, complex composite formulations are required that satisfy the aforementioned requirements, in combination with surface properties that will ensure long-term hydrophobicity to prevent the formation of continuous water films that can cause electrical failures.<sup>1</sup> On top of surface chemistry (hydrophobic), the surfaces of instrument transformers are typically designed to have an undulating shape that prevents the formation of continuous water films and contamination layers as shown in Figure 1.

Besides the bulk and surface performance requirements, the material composition of outdoor insulation systems needs to comply with current and future regulations that restrict the use of specific chemical compounds that pose a threat for the environment. Therefore, we are looking at sustainable material solutions satisfying the aforementioned properties, while at the same time, we investigate the possibilities of having a circular approach for the end-of-life products. Given the fact that these insulating materials are typically thermosetting polymers in their nature to survive the long-term exposure to outdoor conditions, their recyclability is an additional challenge. In this work we discuss various material design approaches, and we show a few examples. These include approaches for bulk material modification and application of coatings. We also discuss methods for characterizing their performance which includes the evaluation of static and dynamic wetting properties, as well as more specific to the application tests, such as the measurement of leakage currents, tracking and erosion, etc.<sup>2</sup> Based on such measurements we define what experimental outcomes are desired for a material to be considered as a good performing outdoor electrical insulator. The benefit of using self-healing materials is also discussed.

Finally, we also analyze potential recycling strategies of decommissioned products, that so far are typically sent for landfilling or being incinerated. We discuss how this could contribute towards a circular economy and responsible waste management.

**Keywords**: outdoor electrical insulation, hydrophobicity, coatings, surface engineering, UV resistance, composite, self-healing material.



**Figure 1**: Figure illustrating medium-voltage ABB outdoor instrument transformers.

- 1. Al-Karawi, S., Al-Taie, A. (2023) Insulators Used in Outdoor Power Applications: Materials and Coatings, 6th International Conference on Engineering Technology and its Applications (IICETA)
- Tariq Nazir, M., Khalid, A., Akram, S., Mishra, P., Kabir, I. I., Yeoh, G. H., Toan Phung, B., Wong, K. L. (2023) Electrical tracking, erosion and flammability resistance of high voltage outdoor composite insulation: Research, innovation and future outlook, *Materials Science & Engineering R*, 156, 100757.

## Development of High Performance Polydimethylsiloxane-Multi-walled Carbon Nanotubes (PDMS-MWCNTs) Nanocomposites for Triboelectric Nanogenerator Applications

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#### Abstract:

Triboelectric nanogenerators (TENGs) represent a promising and sustainable method for energy harvesting, owing to their efficient conversion of mechanical energy into electrical energy. This research examines the development and performance enhancement of TENG materials through the fabrication of composites comprising polydimethylsiloxane (PDMS) and unfuntionalized multi-walled carbon nanotubes (MWCNTs) produced via a solution mixing technique using tetrahydrofuran (THF) as solvent. The composite thickness ranged from 0.75 mm to 1.25 mm, while the concentration of MWCNTs varied across five weight percentages: 0 wt%, 0.1 wt%, 0.2 wt%, 0.3 wt%, and 0.4 wt%. Two distinct types of MWCNTs were utilized: those with low aspect ratios and those with high aspect ratios. The results showed that under vertical contact-separation mode of operation, shown in Figure 1, the configuration, characterized by a 0.75 mm thick composite with 0.2 wt% MWCNTs, demonstrated the best enhancements in performance for the two types of MWCNTs. Highaspect-ratio MWCNTs produced a peak-to-peak voltage of 376 V, whereas low-aspect-ratio MWCNTs yielded 312 V. Pure PDMS exhibited peak-to-peak output voltages of 114 V at a thickness of 0.75 mm. Figure 2 presents a comparison between the results of all the tested composites. The integration of MWCNTs enhanced voltage generation efficiency by around 222% relative to pure PDMS, highlighting the potential of PDMS-MWCNT composites for advanced TENG applications such as wearable electronics, selfpowered sensors, and IoT devices.

**Keywords**: Energy harvesting, triboelectric nanogenerators, polydimethylsiloxane, multiwalled carbon nanotubes, nanocomposites, solution mixing technique.



**Figure 1:** Diagram illustrating the contact-separation mode of TENG using the PDMS-MWCNTs as tribopositive material and PTFE as tribonegative material.



**Figure 2**: Bar chart showing the average peak-topeak output voltage achieved in relation to varying weight percentages of MWCNTs for the 0.75 mm thick samples.

- 1. T. Xu, J. Ye, and J.-C. Tan, "Unravelling the Ageing Effects of PDMS-Based Triboelectric Nanogenerators," Advanced Materials Interfaces, vol. 11, no. 19, p. 2400094, 2024.
- B. Herren, V. Webster, E. Davidson, M. C. Saha, M. C. Altan, and Y. Liu, "PDMS Sponges with Embedded Carbon Nanotubes as Piezoresistive Sensors for Human Motion Detection," Nano materials, vol. 11, p. 1740, July 2021.
- K. Okochi and T. Oya, "Unique Triboelectric Nanogenerator Using Carbon Nanotube Composite Papers," Applied Sciences, vol. 14, p. 10030, Jan. 2024. Number: 21 Publisher: Multidisciplinary Digital Publishing Institute.

## Sunlight-Driven Nanostructured Polymer Coatings for Energy-Efficient Smart Surfaces

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#### Abstract:

Nature provides inspiration for the design of nanostructured functional materials that respond dynamically to external stimuli. Among these, molecular photoswitches enable reversible control over biological systems, nanomachines, and self-cleaning surfaces<sup>1</sup>. Previously, we reported a copolymer coating composed of azobenzene unsubstituted and SBMA. demonstrating near-complete cleaning of irreversible fouling by bacteria and BSA protein under UV/visible light activation<sup>2</sup>.

To improve energy efficiency and practicality, we have developed in this study a novel selfcleaning coating by synthesizing a red-lightshifted, crosslinked copolymer incorporating a substituted azobenzene moiety and a zwitterionic segment. We subsequently studied the reversible nanostructural and mechanical changes in the thin film entirely under visible wavelengths (LEDs; green, blue, red) and a lab-scale solar simulator.

The photoresponsive properties of the crosslinked copolymer were systematically characterized through UV-vis spectroscopy, enabling a comprehensive analysis of its spectral and photokinetic behaviour. Atomic force microscopy (AFM) studies revealed highly reversible, light-induced nanoscale morphological and mechanical changes, driven by alternating irradiation with green and blue wavelengths, which predominantly triggered trans-cis and cis-trans isomerization (Figure 1). Furthermore, solar simulator irradiation triggered simultaneous isomerization, resulting in dynamic oscillatory surface changes.

Unlike previous studies, we directly monitored the structural evolution of the same surface area under alternating visible light, revealing precise nanometer-scale transformations. These findings hold significant potential for future development of light-responsive polymer coatings for selfcleaning surfaces powered by energy-efficient visible light or ambient sunlight.

**Keywords**: Light-responsive coatings, solardriven smart materials, azobenzene-based polymers, nanostructured thin films, selfcleaning applications, atomic force microscopy.



Figure 1: AFM images (5  $\mu$ m×5  $\mu$ m) & the corresponding RMS roughness along the white dashed line demonstrate reversible change on surface topography of nanostructured thin film under Green $\Rightarrow$ Blue light irradiation.

- 1. Lee, S., Kang, H. S. (2012) Directional Photofluidization Lithography: Micro/Nanostructural Evolution by Photofluidic Motions of Azobenzene Materials, *Adv. Mater.*, 24, 2069–2103.
- Das, P., Durban-Benizio, N., Desclaux, S., Causserand, C., Remigy, J.-C., Lahitte, J.-F., Pimienta, V., Coudret, C., Coetsier, C. (2024) Light-responsive zwitterionic membrane surface modification for antifouling and antibacterial application, *Chem. Eng. Jour.*, 500, 157337.

# Effect of electron-phonon interaction on thermoelectric properties through DNA chains

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#### Abstract:

The study of nanoscopic systems has further highlighted the potential of biomolecules, such as DNA, as promising candidates for nanoelectronics. DNA, with its unique molecular structure and tunable properties, offers a versatile platform for developing novel electronic devices. Unlike conventional materials, biomolecules present an opportunity to combine biological functionality with electronic applications, paving the way for hybrid systems that leverage the advantages of both domains.

In this context, understanding the transport properties of DNA under different conditions is critical for advancing its application in molecular electronics. Decoherence effects, arising from inelastic interactions such as electron-phonon coupling, play a pivotal role in determining the electronic, thermal, and thermoelectric performance of these systems. Exploring these effects can provide fundamental insights into the mechanisms governing charge and energy transport at the molecular scale.

Therefore, we investigate the thermoelectric properties, considering decoherence effects, of a DNA molecule placed between semi-infinite contacts (Figure 1). Our model incorporates two representations: the Fishbone and Ladder models. Employing the tight-binding approach, we utilize the Green's function technique along with real-space renormalization and polaron transformation schemes. Specifically, we calculate the transmission probability using the Landauer-Buttiker formalism, analyze I-V characteristics, explore electrical conductance, thermal conductance, Seebeck coefficient, figure of merit and Lorenz number, all while accounting for decoherence effects. Our study provides insights into understanding inelastic effects within nanoscopic molecular systems.

**Keywords**: Green's functions, decoherence, thermoelectrics, molecular systems.



**Figure 1**: Panels I: Fishbone model of DNA. (a) Representation for each atomic site, (b) Fishbone model of DNA with N atomic sites, (c) Fishbone model of DNA normalized to an effective strand with N effective sites. Panels II: Ladder model of DNA. (a) Representation for each atomic site, (b) Ladder model of DNA with N atomic sites, (c) Ladder model of DNA normalized to an effective strand with N effective sites.

- 1. S. Datta, (1997) *Electronic Transport in Mesoscopic Systems*, Cambridge University Press: Cambridge.
- J.H. Ojeda, M. Pacheco, L. Rosales and P.A. Orellana. (2012) Current and Shot noise in DNA chains, *Organic Electronics* 13, 1420.
- 3. J.H. Ojeda, C.A. Duque, D. Laroze. (2016) Electron-phonon interaction in quantum transport through quantum dots and molecular systems, *Physica B* **502** 73-81
- Judith Helena Ojeda Silva and Santanu K. Maiti. (2019) Thermal Properties of Ordered and Disordered DNA Chains: Efficient Energy Conversion, *ChemPhysChem* 20, 3346-3353
- M. A. Rivera Mateus, J. H. Ojeda, and D. Gallego. (2020) Thermoelectric properties through a wire composed of isoprene molecules, *AIP Adv.*, vol. 10, no. 6, p. 065021, doi: 10.1063/5.0008266.

## Harnessing Nanotechnology and Plasmonics at the Frontiers of Biomedical Diagnostics

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#### Abstract

This lecture showcases laser-enabled nanoplasmonics research from our laboratory that is redefining the future of medical diagnostics. At the heart of this work is plasmonics—the manipulation of the enhanced electromagnetic properties of metallic nanostructures. These structures interact with incident electromagnetic fields, triggering oscillations of conduction-band electrons—known as surface plasmons—that generate powerful secondary electric fields. This phenomenon, known as surface plasmon resonance, forms the foundation of surface-enhanced Raman scattering (SERS), which enables ultra-sensitive molecular detection.

Our focus lies in harnessing the dynamic interaction between laser light and intricately engineered metallic nanoparticles to amplify SERS signals by a factor of over one million. This plasmonic enhancement marks a transformative leap in biosensing, enabling the detection of disease-related molecules at previously unreachable limits. Central to our technology are laser-activated nanoplatforms with precisely designed nanoscale spikes that emit ultrabright SERS signals. These next-generation sensors redefine sensitivity in diagnostic platforms. We have developed SERS-based nanochip systems capable of detecting DNA biomarkers for various cancers and infectious diseases such as HIV, malaria, and dengue—offering critical advancements in global health diagnostics. We have engineered portable biosensors as "lab-in-a-stick" nanotools for the rapid diagnosis of head and neck cancers. Our expanding platform includes plasmonics-enhanced lateral flow immunoassays, smartphone-integrated biosensors, and implantable "smart tattoo" systems—each offering new capabilities for accessible, point-of-care diagnostics.

Most significantly, our nanoplasmonic biosensors can detect disease-specific biomarkers directly, without requiring lab-based PCR amplification. This capability is critical for early diagnosis—often before symptoms appear—enabling timely intervention and improving patient outcomes. With built-in multiplexing and high sensitivity to molecular and genomic biomarkers, our plasmonic detection platforms are poised to elevate precision medicine, transforming how we detect, monitor, and treat disease across the globe. These technologies open new frontiers in medical testing: rapid, low-cost, non-invasive, and deployable in both clinical and remote settings.

## Nanotech France / GAMS 2025 Joint Session II. B: Nano for life science and Medicine

## Scalable Microfluidic Synthesis of PEGylated Liposomes for Drug Delivery and Cosmetic Applications

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#### Abstract:

Liposomes are versatile nanocarriers with promising applications in both targeted drug delivery and cosmetics. Despite their potential in drug delivery and cosmetics, the clinical and commercial translation of liposomes is hindered by challenges in scalability, reproducibility, and size control during synthesis. Conventional methods such as ethanol injection and thin-film hydration often lead to inconsistent size distribution and poor encapsulation efficiency [1, 2]. In this study, we present a high-throughput microfluidic platform synthesizing for PEGylated liposomes with high reproducibility and precise control over size distribution. This platform enables the one-step generation of homogeneous liposomes while simultaneously encapsulating a hydrophobic cargo during the self-assembly process (Figure 1). The effects of key parameters, including chip geometry, total flow rate, flow rate ratio, lipid concentration, and solvent-buffer composition, were systematically investigated to fine-tune liposome size and polydispersity. Our approach enables precise control over liposome sizes ranging from 60 nm to 150 nm, with a polydispersity index (PDI) of less than 0.2 [1].

We synthesized two types of liposomes with distinct mechanical properties: low-rigidity liposomes using egg yolk phosphatidylcholine (Egg-PC) and high-rigidity liposomes using 1,2distearoyl-sn-glycero-3-phosphocholine

(DSPC), high-transition-temperature а phospholipid. To ensure reproducibility, a temperature-controlled synthesis platform was for DSPC-based implemented liposomes. Encapsulation efficiency was evaluated using Nile Red as a surrogate hydrophobic drug, achieving up to 74% encapsulation efficiency. The encapsulation process occurs within the microfluidic chip during the self-assembly of liposomes, offering a scalable and reproducible method for generating liposomes suitable for both therapeutic and cosmetic formulations. Future work will explore the application of these liposomes in transdermal drug penetration and cosmetic formulations, addressing the growing need for customizable, on-demand nanocarrier systems in medicine and skincare.

**Keywords**: Microfluidics, PEGylated liposomes, drug delivery, cosmetic formulations, encapsulation efficiency



Figure 1: The schematics of liposome preparation on a microfluidic chip **References:** 

[1] Akar S, Fardindoost S, Hoorfar M. High throughput microfluidics-based synthesis of PEGylated liposomes for precise size control and efficient drug encapsulation. Colloids and Surfaces B: Biointerfaces. 2024 Jun 1;238:113926.

[2] Dangkoub F, Naeini MB, Akar S, Badiee A, Jaafari MR, Sankian M, Tafaghodi M, Shaegh SA. Preparation of atorvastatin calcium-loaded liposomes using thin-film hydration and coaxial micromixing methods: A comparative study. International Journal of Pharmaceutics: X. 2024 Dec 1:8:100309.

## Molecular Dynamics in Nanomedicine: From Molecular Insights to Functional Design

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#### Abstract:

Molecular dynamics (MD) methods have become indispensable tools in the rapid advancement of nanomedicine. These techniques computational offer unique capabilities for the detailed characterization of molecular processes, effectively complex complementing and extending traditional experimental approaches. In this talk, I will showcase how advanced MD simulations not only support experimental findings but also push the boundaries of the rational design of bioinorganic nanohybrid materials by uncovering critical molecular behaviors that are often beyond the reach of conventional experiments. Through a series of case studies — including (1) the influence of thermodynamic variables (e.g., pH and ionic strength) on protein corona formation around bio-functionalized metal oxide nanoparticles<sup>1</sup>, (2) the design of specific lipidbased nanocarrier compositions for enhanced anti-tumor drug delivery<sup>2</sup>, and (3) the characterization of self-assembled organic monolayers coating gold and magnetite nanoparticles<sup>3</sup> — this presentation will highlight the integration of MD simulations with experiments as a powerful approach to bridging the gap between microscopic molecular behavior and macroscopic functionality.

**Keywords**: nanomedicine, bio-inorganic nanohybrids, protein corona, free energy, drug delivery, self-assembled monolayers, polymer coating, molecular dynamics, nanoparticles.



**Figure 1**: Formation of the hard protein corona around a bio-functionalized titanium dioxide metal oxide nanoparticle immersed in physiological solution, modeled and simulated at the atomistic level using Molecular Dynamics techniques

- 1. Siani, P., & Di Valentin, C. (2022). *Nanoscale*, 14(13), 5121–5137.
- Siani, P., Donadoni, E., Ferraro, L., Re, F., & Di Valentin, C. (2022). *Biochimica et Biophysica Acta, Biomembranes*, 1864(1), 183763.
- Siani, P., Bianchetti, E., & Di Valentin, C. (2025). *npj Computational Materials*, 11(1), 20.

## Mycosynthesis, Characterization, and Mosquitocidal Activity of Silver Nanoparticles Fabricated by Aspergillus niger Strain

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Mahmoud H. Sultan 2 , Samy Selim 5 , Areej A. Al-Khalaf 6 and Amr Fouda 2,\*

Author/presenter: Prof Areej Al-khalaf

#### Abstract:

Herein, silver nanoparticles (Ag-NPs) were synthesized using an environmentally friendly approach by harnessing the metabolites of Aspergillus niger F2. The successful formation of Ag-NPs was checked by a color change to yellowishbrown, followed by UV-Vis spectroscopy, Fourier transforms infrared (FT-IR), Transmission electron microscopy (TEM), and X-ray diffraction (XRD). Data showed the successful formation of crystalline Ag-NPs with a spherical shape at the maximum surface plasmon resonance of 420 nm with a size range of 3-13 nm. The Ag-NPs showed high toxicity against I, II, III, and IV instar larvae and pupae of Aedes aegypti with LC50 and LC90 values of 12.4-22.9 ppm and 22.4-41.4 ppm, respectively under laboratory conditions. The field assay exhibited the highest reduction in larval density due to treatment with Ag-NPs (10× LC50) with values of 59.6%, 74.7%, and 100% after 24, 48, and 72 h, respectively. The exposure of A. aegypti adults to the vapor of burning Ag-NPsbased coils caused a reduction of unfed individuals with a percentage of  $81.6 \pm 0.5\%$  compared with the positive control, pyrethrin-based coils (86.1  $\pm$  1.1%). The ovicidal activity of biosynthesized Ag-NPs caused the hatching of the eggs with percentages of 50.1  $\pm$  0.9, 33.5  $\pm$  1.1, 22.9  $\pm$  1.1, and 13.7  $\pm$ 1.2% for concentrations of 5, 10, 15, and 20 ppm, whereas Ag-NPs at a concentration of 25 and 30 ppm caused complete egg mortality (100%). The obtained data confirmed the applicability of biosynthesized Figure 2. FT-IR spectra of fungal biomass filtrate (A) and Ag-NPs fabricated by Aspergillus niger strain F2 (B).Ag-NPs to the biocontrol of A. aegypti at low concentrations

**Keywords**: biosynthesis; silver nanoparticles; biocontrol; larvicidal; smoke toxicity; ovicidal



**Figure 1.** Color change and UV-Vis spectroscopy analysis of mycosynthesized Ag-NPs at wavelengths of 300–600 nm.



**Figure 2.** FT-IR spectra of fungal biomass filtrate (A) and Ag-NPs fabricated by *Aspergillus niger* strain F2 (B).



Figure 3. Characterization of Ag-NPs formed by biomass filtrate of *A. niger* strain F2. (A) is the TEM image, and (B) is the size distributions based on the TEM image.

- Soliman, A.M.; Abdel-Latif, W.; Shehata, I.H.; Fouda, A.; Abdo, A.M.; Ahmed, Y.M. Green Approach to Overcome the Resistance Pattern of Candida spp. Using Biosynthesized Silver Nanoparticles Fabricated by *Penicillium chrysogenum* F9. *Biol. Trace Elem. Res.* 2021, 199, 800–811. [Google Scholar] [CrossRef] [PubMed]
- Manimegalai, T.; Raguvaran, K.; Kalpana, M.; Maheswaran, R. Green synthesis of silver nanoparticle using *Leonotis nepetifolia* and their toxicity against vector mosquitoes of *Aedes aegypti* and *Culex quinquefasciatus* and agricultural pests of *Spodoptera litura* and *Helicoverpa armigera*. *Environ*. *Sci. Pollut. Res. Int.* 2020, 27, 43103–43116. [Google Scholar] [CrossRef] [PubMed]
- Shaheen, T.I.; Fouda, A.; Salem, S.S. Integration of Cotton Fabrics with Biosynthesized CuO Nanoparticles for Bactericidal Activity in the Terms of Their Cytotoxicity Assessment. *Ind. Eng. Chem. Res.* 2021, 60, 1553–1563. [Google Scholar] [CrossRef]

### A New bone nano-hemostatic agent with antibacterial activity

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#### Abstract:

Bleeding may easily cause death during surgery. Most recent topical hemostatic agents demonstrated to control bone bleeding ineffectively and increase the rate of surgical site infection. Searching among biosynthesized nanoparticles (NPs) has promising result. The aim of this study is to investigate the physicochemical and biological properties of prepared silver nanoparticles from Urtica dioica (UD-AgNPs) and to test their potential effect as a bone hemostatic agent. Silver nanoparticles (AgNPs) were synthesized using ethyl acetate extract from Urtica dioica (UD) leaves. UD-AgNPs were characterized using ultravioletvisible spectroscopy, energy-dispersive X-ray analysis, fourier transform infrared spectroscopy, X-ray diffraction, dynamic light scattering, transmission electron microscopy, and scanning electron microscopy. UD-AgNPs were assessed against Gram-positive and Gram-negative bacteria. The active components of the ethyl acetate extract were identified by gas chromatography-mass spectrometry (GC-MS). MTT assay performed to evaluate UD-AgNPs cytotoxicity against normal and cancerous cells. Under general anesthesia, two circular defects 3 mm in diameter were created on the right femur of each rat. In group I: defect left unfilled ( negative control); in groups II, III, and IV: defects were filled with bone wax, Surgicel® and UD-AgNPs, respectively. Bleeding time and blood loss was evaluated in each group. Further, coagulation profile and complete blood count were tested at baseline, one week and four weeks postoperatively. The NPs were 19.401 nm in size, spherical and negatively charged the UD-AgNPs surface. The zone of inhibition for 75 µL of UD-AgNPs against Pseudomonas aeruginosa was 21  $\pm$  0.4 mm more than control drug Ciprofloxacin  $(16 \pm 10 \text{ mm})$ . The minimum inhibitory concentration was the lowest against Escherichia coli  $(36 \pm 3 \mu g/mL)$  and Staphylococcus epidermidis (38  $\pm$  3  $\mu$ g/mL). The minimum bactericidal concentration was the lowest against Escherichia coli  $(75 \pm 00 \ \mu g/mL)$  and Enterococcus faecalis ( $83 \pm 16 \mu g/mL$ ). GC-MS shows active components used in bleeding control and antibacterial activities like Phytol, Neophytadiene and Carboxylic acid. MTT assay showed cell viability higher than 75% in all UD-AgNPs concentrations against

normal cells. UD-AgNPs revealed immediate hemostasis (7.7 second) almost like bone wax (7.3 second) with similar amount of blood loss (0.05 gm). UD-AgNPs increased PLT (1347.5×103 /uL), reduced aPTT (12.6 second) and keep normal WBC comparing to bone wax (19.2×103 /uL) at first week. These observations suggested UD-AgNPs as an effective hemostatic agent with antibacterial activity.

**Keywords**: UD-AgNPs; Characterization; Green synthesis; Antimicrobial effects, UD-AgNPs; hemostasis; bone bleeding; cytotoxicity, In-vitro and In-Vivo



**Figure 1**: Figure illustrating the synthesis of UD-AgNPs and its application as antibacterial and bone hemostatic agent.

- Dikshit, P. K., Kumar, J., Das, A. K., Sadhu, S., Sharma, S., Singh, S., ... & Kim, B. S. (2021). Green synthesis of metallic nanoparticles: Applications and limitations. Catalysts, 11(8), 902.
- Devanesan, S., & AlSalhi, M. S. (2021). Green synthesis of silver nanoparticles using the flower extract of Abelmoschus esculentus for cytotoxicity and antimicrobial studies. International Journal of Nanomedicine, 3343-3356.
- Rama, P., Baldelli, A., Vignesh, A., Altemimi, A. B., Lakshmanan, G., Selvam, R., ... & Pratap-Singh, A. (2022). Antimicrobial, antioxidant, and angiogenic bioactive silver nanoparticles produced using Murraya paniculata (L.) jack leaves. Nanomaterials and Nanotechnology, 12, 18479804211056167.

## Multifunctional properties of Dy<sub>2</sub>O<sub>3</sub>-Doped ZnO nanoparticles: Optical, dielectric, and antibacterial performance

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#### Abstract:

Antibiotics and antifungals have significantly advanced healthcare by enabling the effective treatment of infectious diseases. However, the increasing prevalence of antimicrobial resistance (AMR), driven by mechanisms such as enzymatic degradation and altered membrane permeability, has emerged as a critical global concern. Drug-resistant pathogens, including *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and *Klebsiella pneumoniae*, are responsible for severe infections like pneumonia and sepsis, emphasizing the urgent need for innovative therapeutic strategies [1].

Nanotechnology, particularly the use of metal and metal oxide nanoparticles, presents a promising approach to combating AMR. ZnO nanoparticles have garnered considerable attention due to their biocompatibility, costeffectiveness, and potent antibacterial properties [3]. Doping ZnO with metal or non-metal elements has been shown to enhance its antibacterial and photocatalytic performance by modifying its electronic structure, introducing structural defects, and increasing the generation of reactive oxygen species (ROS) [2]. These ROS disrupt bacterial membranes, inhibit microbial growth, and contribute to the photocatalytic degradation of organic pollutants.

In this study, Dy<sub>2</sub>O<sub>3</sub>-doped ZnO nanoparticles were synthesized using a solid-state method to enhance their multifunctional properties for electronic and biomedical applications. Structural, optical, and dielectric characterization using X-ray diffraction (XRD), scanning electron microscopy (SEM), UV-Vis diffuse reflectance spectroscopy, and dielectric spectroscopy confirmed notable improvements. XRD analysis revealed the coexistence of wurtzite ZnO and minor Dy<sub>2</sub>O<sub>3</sub> phases, maintaining structural integrity as physical mixtures. Optical studies indicated a slight bandgap narrowing from 3.3 eV to 3.2 eV, suggesting improved electronic performance. Dielectric measurements showed enhanced conductivity and reduced dielectric losses at high frequencies, reinforcing the material's potential for advanced electronic applications. Furthermore, antibacterial assays demonstrated significant activity against Pseudomonas aeruginosa, particularly in surfactant-containing environments, underscoring Dy:ZnO's effectiveness as an antimicrobial agent against gram-negative bacteria.

**Keywords**: nanoparticles; antibacterial activity; Zinc Oxide; Dysprosium oxide; dielectric properties.

- 1. https://www.who.int/news/item/27-02-2017
- W.Y. Belay, M. Getachew, B.A. Tegegne, Z.H. Teffera, A. Dagne, T.K. Zeleke, R.B. Abebe, A.A. Gedif, A. Fenta, G. Yirdaw, A. Tilahun, Y. Aschale, Mechanism of antibacterial resistance, strategies and nextgeneration antimicrobials to contain antimicrobial resistance: a review, Front. Pharmacol. 15 (2024). https://doi.org/10.3389/fphar.2024.1444781.
- 3. J. Jiang, J. Pi, J. Cai, The Advancing of Zinc Oxide Nanoparticles for Biomedical Applications, Bioinorganic Chemistry and Applications 2018 (2018) 1062562. https://doi.org/10.1155/2018/1062562.

## Mn-Doped Carbon Dots as MRI Contrast Agents: Insights from Phantom Studies toward Neuroimaging Use

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#### Abstract:

Manganese-doped carbon dots (Mn-CDs) have recently emerged as versatile nanostructures with promising applications in biomedical imaging.

Usually,  $Mn^{2+}$  works similarly as other paramagnetic ions, like  $Gd^{3+}$  and  $Cu^{2+}$ , able of shortening the T1 of water protons, thus increasing the signal of T1w MR images, but also exhibit a modest T2 effect, by reducing the signal intensity to produce dark signals. [1]

In the current work, different Mn-CDs were synthesized and characterized using spectroscopic (UV-Vis, XPS), FTIR. morphological (STEM), and elemental analysis (EDX) techniques. The resulting nanoparticles displayed high aqueous stability, narrow size distribution (5-20 nm depending on synthesis parameters) and surface functionalities favorable for biological applications. Their MRI contrast properties were investigated through phantom imaging in 1% agarose gel at 1 T field strengths on a nanoScan PET-MRI equipment (Mediso, Hungary), for small animals.

In T1w GRE sequences the signal enhancement was highly dependent on the flip angle (FA), with minimal contrast at small FA, whereas strong signal enhancement was recorded at higher FA, due to an effective T1 shortening effect. In T2w FSE sequences, a clear echo time (TE)dependent contrast inversion was observed. At reduced TE, regions containing Mn-CDs exhibited increased signal intensity, suggestive of residual T1 contribution and insufficient T2 decay. By increasing TE, a transitional behavior was noted, with decreasing signal intensity, reaching at higher TE pronounced signal attenuation, consistent with dominant T2 shortening effects. These observations correlate well with the relaxivity values measured for the nanoparticles, yielding an  $r_2/r_1$  ratio higher than 5, which classifies them as T2-dominant contrast agents.[2] The dual-mode response observed in both imaging regimes underscores their potential versatility for MRI applications, particularly in T2w contrast enhancement at clinically relevant field strengths.

Such behavior suggests that Mn-CDs may act predominantly via magnetic susceptibility effects rather than classical paramagnetic relaxation, highlighting their unique mechanism of contrast enhancement. These findings align with recent trends exploring carbon-based nanomaterials for MRI and provide novel insights into the design of dual-mode or tunable MRI agents.

Given their small size, biocompatibility, ease of synthesis, and feasible MRI contrast effect, Mn-CDs represent promising candidates for further development in neuroimaging, particularly for preclinical studies focused on early detection of neurodegenerative disorders.

**Keywords**: Carbon Dots, MRI contrast agents, diagnosis, relaxivity



**Figure 1**: The contrast behaviour of a Mn-CDs formulation in MR imaging highlighting the influence of FA and TE on the image brightness.

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- 1. Pan, D., Schmieder, A.H., Wickline, S.A., Lanza, G.M. (2011) Manganese-based MRI contrast agents: past, present and future, *Tetrahedron*, 67(44), 8431–8444
- Caspani, S., Magalhães, R., Araújo, J.P. Sousa, C.T. (2020) Magnetic Nanomaterials as Contrast Agents for MRI, *Materials*, 13, 2586, 1-29

## DEVELOPMENT OF STABLE BIOFUNCTIONALIZED PET MEMBRANES, WITH BIOACTIVE BINDING POINTS, FOR POTENTIAL APPLICATION IN CELL CULTURING DEVICES

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#### Abstract:

Although some commercially available membranes have shown good results and many approaches have been employed to further improve their ability to promote cell binding, by mimicking the extracellular microenvironment, still some issues arise regarding inter-batch variability, uncontrolled degradation, and absence of bioactive binding points, which urge the need for a proper functionalization. Thus, our approach involved the introduction of functional groups (-COOH) on the surface of porous PET membranes, that can facilitate the covalent binding of cellular ligands.

The tested membranes had different pore sizes and orientations. All the membranes have been cleaned and dried, after which subjected to hydrolysis.

Membrane characterization was carried out by Toluidine Blue O (TBO) staining assay, scanning electron microscopy (SEM) and Fourier Transform Infrared Spectroscopy (FT-IR). The TBO assay revealed that the chemically treated membrane had the largest density of -COOH groups. The SEM images suggest that the surface was not damaged during the chemical treatments, however, there was a significant change in the pore size, from around 520-550 nm to 1.5-1.8 um. By comparing the FT-IR spectra of the untreated membrane with the samples subjected to the four chemical treatments, there is a sharp decrease of the spectral bands in the region 1800-700 cm-1 and slight modifications in the 4000-2800 cm-1 region. In the region 4000-2800 cm-1, the FT-IR spectra show wider bands centered at about 3360 cm-1, bands that can be associated with the vibrational mode characteristic of OH bonds and overlapping the bands associated with the stretching vibration of CH bonds in the PET structure.

To assess the protein immobilization capacity of the newly functionalized membrane, the Green Fluorescent Protein (GFP) was used. The protein was immobilized via covalent binding. Fluorescence microscopy images obtained with Axio Observer D1 microscope revealed good distribution of the protein on the in-house functionalized membrane, comparable to the commercially available ones (Fig. 1). FT-IR, EDX and SEM analysis confirm the presence of the protein and the modification of surface roughness.

The newly functionalized membranes showed promising results, as potential substrate for the desired application. Future studies involve the immobilization of cell ligand molecules, that will ensure optimum cell adhesion, with the completion of all 3 adhesion stages: i) initial physico-chemical contact; ii) integrins attachment and cell spreading initiation; iii) final spreading stage.

**Keywords**: membrane, protein, functional groups, cell adhesion.



**Figure 1**: Fluorescent images of the membrane: A) without GFP, B) with GFP

#### Acknowledgements:

This work is founded by the UNLOOC project supported by the Chips Joint Undertaking and its members Belgium, Germany, Hungary, Ireland, Italy, the Netherlands, Portugal, Romania, Spain, Switzerland. Grant Agreement No. 101140192. A grant of the Romanian Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-IV-P8-485, 21/2024 and co-financed by DDS Diagnostic.

- Pratt, K. J., Williams, S. K., & Jarrell, B. E. (1989). Enhanced adherence of human adult endothelial cells to plasma discharge modified polyethylene terephthalate. J. Biomed. Mater. Res., 23(10), 1131–1147.
- Ramachandran, B., Chakraborty, S., Dixit, M., & Muthuvijayan, V. (2018). A comparative study of polyethylene terephthalate surface carboxylation techniques: Characterization, in vitro haemocompatibility and endothelialization. React. Funct. Polym., 122, 22–32.

## Sol-Gel Synthesis of Silica-based Biomaterials containing Rosmarinic Acid and Polyethylene Glycol

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#### Abstract:

One technique used for the synthesis of a wide range of materials, including biomaterials, is the sol-gel technique, which involves the formation of a sol (a colloidal dispersion of solid particles in a liquid) which is then transformed into a gel (a cross-linked three-dimensional solid structure) through polymerization or cross-linking processes. Implanted biomedical devices can cause adverse responses in the human body, such as infections and inflammation, which can lead to implant failure. Today, natural products are one of the main sources of new pharmaceutical molecules that can prevent illnesses and/or inflammations. The sol-gel process has been used in the biomaterials industry to create materials with certain properties that are appropriate for a range of biomedical uses, including tissue engineering, drug delivery, and tissue regeneration. The creation of biomedical with implants anti-inflammatory and antibacterial qualities via sol-gel synthesis is the goal of this project (Fig. 1). Different weight percentages (5, 10 and 15<sub>wt</sub>%) of Rosmarinic Acid (RA) and different weight percentages (6, 12 and 24<sub>wt</sub>%) of Polyethylene Glycol (PEG) were incorporated into the silica matrix (SiO<sub>2</sub>). Rosmarinic acid is a phenolic compound present in several plants, including rosemary (from which it takes its name), sage and lemon balm. The interactions between different organic and inorganic phases in the hybrid materials were studied using Fourier transform spectroscopy infrared (FTIR). The biocompatibility of SiO<sub>2</sub> and SiO<sub>2</sub>/RA/PEG evaluated. were indicating that these synthesized materials did not induce cell toxicity. Furthermore, the antimicrobial activity of SiO<sub>2</sub> and SiO<sub>2</sub>/RA/PEG was tested against Escherichia coli (E. coli) and antioxidant activity was evaluated by the FRAP method.

**Keywords**: Sol-gel glasses, silica-based biomaterials, rosmarinic acid, biomedical applications.



Figure 1: Sol-gel procedure used to obtain hybrid materials under study

- Barrino, F. (2024). Hybrid Organic– Inorganic Materials Prepared by Sol–Gel and Sol–Gel-Coating Method for Biomedical Use: Study and Synthetic Review of Synthesis and Properties. *Coatings*, 14(4), 425.
- Noor, S., Mohammad, T., Rub, M. A., Raza, A., Azum, N., Yadav, D. K., ... & Asiri, A. M. (2022). Biomedical features and therapeutic potential of rosmarinic acid. Archives of Pharmacal Research, 45(4), 205-228.
- Catauro, M., Barrino, F., Dal Poggetto, G., Pacifico, F., Piccolella, S., & Pacifico, S. (2019). Chlorogenic acid/PEG-based organic-inorganic hybrids: A versatile solgel synthesis route for new bioactive materials. *Materials Science and Engineering: C*, 100, 837-844.

## Non-Invasive Label-Free Electrical and Optical Parrallel Recordings of Electrophysiological Action Potentials of hiPSC Cardiomyocytes

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#### Abstract:

Among the many molecules tested every year as potential drugs, 90% fail to reach the market despite sometimes more than 12 years of development and over two billion individual costs. As rejections are often related to cardiovascular issues, some cell-lines such as hiPSC cardiomyocytes have been extensively used to model drug toxicity in vitro, translating efficiently to clinical trials afterward. However, at the current state of art, parameters such as mechanical contractility, electrophysiological signals and calcium fluxes must be measured separately, on different types of devices and often on different in vitro cultures. This makes the interpretation of results difficult and therefore reduces their relevancy. In that context, we developed a novel device that: i) is able to optically record electrophysiological signals in a label-free and non-invasive manner. ii) has embedded electrodes for direct recordings of field potentials and for cell stimulation at the electrode location iii) is transparent enough to enable calcium imaging using fluorescence microscopy. Moving beyond the simple sum of these data, the device couples these modes that can be used independently and simultaneously. Thus, it provides a platform on which relevant and time-efficient studies of cardiotoxicity can be performed. One can use electrodes to pace the surrounding cells and detect discrepancies in cardiac frequency due to assayed drugs. The cardiotoxic effect can be detected at the whole culture level using the high-density optical sensors. In this work, we could observe for example the modification induced bv isoprenaline in action potential duration and frequency. To conclude, this device exploits and combines microfluidics, fluorescent dyes, complex nanofabrication and pass-through electrodes to transduce the cardiac action potentials into optical signals. Using the same structure, it can also perform basic electrical recordings and stimulation, allowing deep studies of drugs cardiotoxicity, necessary to improve drug approval rates.

**Keywords:** biosensor, cardiomyocyte, contractility biomedical engineering,

nanofabrication, membranes, multi-electrode array, label-free detection.



Figure 1: SEM image showing the all-in-one microstructures used on TOXFREE devices to detect in a label-free, non-invasive manner, and at whole culture scale, the contraction of hiPSC cardiomyocytes. On some of the structures, electrodes functionality is embedded as seen at the center. Scale bar 50  $\mu$ m.

## Homogenously-sized PLGA-encapsulated chlamydial protein is efficiently delivered into dendritic cells by activating the caveolin endocytosis pathway to boost innate immune responses

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#### Abstract:

The current study sought optimize to microfluidic fabrication parameters for sizetunable biodegradable polymeric nanoparticles (BPNs) to elucidate the effect of homogenous nanoparticle size on targeted therapeutic delivery of proteins. Previously, we employed PLGA (poly D, L-lactide-co-glycolide) BPNs for intracellular targeting of a modeled chlamydial recombinant major outer membrane protein (rMOMP). Utilizing microfluidics technology, we fabricated small (80 nm) and homogenously (PDI 0.067) PLGA-rMOMP-SHM sized (Staggered herringbone micromixer) BPNs. Herein, we aim to optimize the fabrication of microfluidic BPNs with tunable size to investigate the effect of size on cellular internalization and immune responses. Through the alteration of microfluidic parameters, including total flow rate (TFR), flow rate ratio (FRR), and organic phase PLGA concentration, we fabricated rMOMP-encapsulated BPNs within desired size thresholds of sub-100 nm (small), 150-200 nm (medium), and 200-300 nm (large). These small, medium, and large PLGArMOMP-SHM BPNs were physical-structurally characterized utilizing zeta-size, zeta-potential, UV-vis spectrometry, FT-IR, and SEM, revealing that the fabricated BPNs fell within their desired size ranges, were homogenously sized (PDI<0.1), and efficiently encapsulated the rMOMP. The in vitro stimulation of mouse bone marrow-derived dendritic cells (DCs) at different concentrations (0.1, 1, and 5  $\mu$ g/ml) showed that microfluidics-based homogenous encapsulated rMOMP formulations activated the caveolin endocytosis pathway and induced pattern recognition receptor, co-stimulatory, molecules, and cytokines immune responses at higher levels than the conventional heterogenous encapsulated rMOMP. Overall, microfluidics homogenouslysized encapsulated protein formulations are more efficient for targeted delivery and boosting immune responses than conventional heterogeneous formulations bv activating specific endocytosis pathways.

**Keywords**: Microfluidics, Caveolin, Protein delivery, PLGA nanoparticles.



**Figure 1**: Illustration of TNF- $\alpha$  cytokine production in dendritic cells stimulated by microfluidics homogenous and conventional heterogeneous PLGA-encapsulated chlamydial protein.

- Sahu R, Dixit S, Verma R, Duncan SA, Coats MT, Giambartolomei GH, Singh SR, Dennis VA: A nanovaccine formulation of Chlamydia recombinant MOMP encapsulated in PLGA 85:15 nanoparticles augments CD4(+) effector (CD44(high) CD62L(low)) and memory (CD44(high) CD62L(high)) T-cells in immunized mice. Nanomedicine 2020, 29:102257.
- 2. Roces CB, Christensen D, Perrie Y: Translating the fabrication of protein-loaded poly(lactic-co-glycolic acid) nanoparticles from bench to scale-independent production using microfluidics. *Drug Deliv Transl Res* 2020, 10:582-593.

## Nanotech France/ GAMS 2025 Joint Session III: Nano for life science and Medicine

## Unlocking Non-parenteral Routes: Nanocarrier Systems for Biological Therapeutics

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#### Abstract:

The large surface area of the lungs with the thin epithelial membrane and dense vasculature makes lung delivery a suitable route of administration of biopharmaceuticals for local or systemic targets. Delivery of biologicals such as therapeutic proteins, vaccines, genes etc, to the lungs has many challenges. This includes, overcoming the biological barriers at sites of administration and action, recognition and elimination by immune system, stability of the Nanocarriers provide platforms to drug. overcome these challenges with better outcomes. However, formulation methods of nanocarriers face many challenges and is a critical factor, which can affect their physicochemical properties on the pharmacokinetics or the therapeutic effects.

We have developed polymer-based nanocarrier systems incorporating biologicals (miRNA, vaccine candidates, antimicrobial peptides). Furthermore, we have incorporated these into dry powder microcarriers using spraydrying technology suitable for lung delivery. We have managed to retain biological stability and activity of biopharmaceuticals, and nanocarrier size following redispersion after spraydrying, and performed aerosolisation studies demonstrating suitability for lung delivery. We have applied the technology in the treatment and management of local lung diseases (COPD, lung infections) and vaccination

## Fish Scales Derived Bioapatite and it's Nanotoxicity on Development of Zebrafish Embryo

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#### Abstract:

The fish scales have a huge unexplored potential for value addition as it contains cardinal molecule, hydroxyapatite (HAp), that finds its applications in various areas of research. This study investigates the extraction. characterization, and toxicity of calcined fish scales at 900°C and then ball milled to obtain bioapatite nanoparticles (bHAp). Synthetic HAp bHAp and of Cyprinus carpio and Ctenopharyngodon idella were characterized using XRD, FTIR, TGA & FESEM. Developmental toxicity in zebrafish at lethal and sublethal concentrations i.e.,  $1600 \text{ mg/L} (LC_{50})$ ; 533 mg/L (1/3<sup>rd</sup> of LC<sub>50</sub>) and 266 mg/L (1/6th of  $LC_{50}$ ) were studied under stereo and confocal microscopes. The XRD patterns confirmed bioapatite as the dominant phase and betatricalcium phosphate as a minor phase. FTIR revealed functional groups (OH<sup>-</sup>, PO<sub>4</sub><sup>3-</sup>, CO<sub>3</sub><sup>2-</sup>) similar to bone apatite while TGA indicated thermal stability up to 500°C. FESEM images showed rough, polygonal shapes with Cyprinus carpio (common carp) having average size of 260±96 nm and *Ctenopharyngodon idella* (grass Carp) is 181±40 nm and synthetic HAp is 142±22nm. Toxicological analysis using stereozoom and confocal microscopy revealed that synthetic hydroxyapatite nanoparticles caused developmental abnormalities, including pericardial edema, yolk sac edema, axial curvature in dose and time-dependent manner. The bioapatite nanoparticles from common carp scales induced minor developmental delays and pigmentation loss, whereas grass carp scale derived bioapatite showed no significant toxicity. Genotoxicity assessment of synthetic hydroxyapatite nanoparticles exposed larvae showed significant DNA damage and apoptosis, especially in the head and eye regions. Therefore, present study highlights the significance of using bHAp in comparison to synthetic HAp nanoparticle for implant material thus, bHAp can be a better alternative in the biomedical fields.

**Keywords**: Nanotoxicity, Bioapatite Nanoparticles, Zebra Fish, Genotoxicity, Particle Size, Biomedical Applications.



**Figure 1**: Bioapatite Powder Nanotoxicity on the Developmental stages of Zebrafish.

- 1. Matiyal, B., Sharma, H., Kumar, N. and Ravneet (2021) Microstructure and biocompatibility of biphasic ceramic (HA/ $\beta$ -TCP) from scales of fresh water fish common carp (*Cyprinus carpio*) (2021). Materials Letters, 304
- Kovrižnych, J. A., Sotníková, R., Zeljenková, D., Rollerová, E., Szabová, E., & Wimmerová, S. (2013). Acute toxicity of 31 different nanoparticles to zebrafish (*Danio rerio*) tested in adulthood and in early life stagescomparative study. *Interdisciplinary toxicology*, 6(2), 67-73.
- 3. OECD (2013), Test No. 236: Fish Embryo Acute Toxicity (FET) Test, OECD Guidelines for the Testing of Chemicals, Section 2, OECD Publishing, Paris.

## Novel Nanoformulations for Breast Cancer Drug Delivery Nanocarriers, Bone Regeneration Scaffolds and Industrial Applications

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#### Abstract:

Tumor targeting of therapeutic or imaging agents has the advantage of improving specificity and effectiveness of treatment for various cancer types. This goal is achieved by using targeted nanoparticles (NPs), however, little is known about their in-vivo tissue distribution. Our latest innovative methods on designing different types of polymer nanocomposite systems and nanoscaffolds that exhibit unique properties in facilitating the successful delivery of drugs to cells as well as help in rapid healing and cell growth will be presented. Core-shell silver-based nanoparticles (Ag NPs), composed of Ag core coated with three different polymeric shells and loaded with chemotherapeutic anticancer drug doxorubisin (DOX) will be presented. Notably, low dosage of targeted drug delivery nanocarriers (NCs) exhibited a synergic anticancer activity, and we believe that the prepared NPs-based combinatorial therapy showed a significant enhanced cytotoxic effect against MCF-7 breast cancer cells.

In addition, a simple and rapid method for radiolabeling of three types of Ag NPs has been performed using  $^{125}$ I isotope, with high labeling yields, >90% without disturbing the optical properties, to be used for specific targeting of cancer cells *in-vivo* will be presented.

In order to monitor the *in-vivo* tissue uptake of radiolabeled Ag NPs using  $\gamma$ -rays, Ag-based radioiodo-NPs with a maximum labeling yield were intravenously injected in normal and solid tumor bearing mice. The preliminary biodistribution study revealed that this new radioiodo-NPs have a high affinity to be localized in the tumor site for a long period of time. The reported highly efficient method provides an extensively useful tool for guidance of design and development of new radiolabeled Agbased NPs as tumor-specific agents for both diagnostic and therapeutic applications.

**Keywords**: drug delivery, cancer, biomaterials, antibacterial, electrospinning, nanofibers, biomedical applications.

Electrospun Nanofiber scaffolds composed of different types of polymers (PVA, PCL, etc) incorporating different natural extracts or drugs and their use and *in-vitro* biological evaluation in antibacterial and bone regeneration studies will be presented. The unique antioxidant activity, the total phenolic content (TPC) of the fabricated nanoscaffolds, in addition to their controlled porosity and degradation and significant improvement in cell proliferation and cell attachment will be presented.



**Figure 1**: Scheme of the synergic cytotoxic effect of radiolabeling DOX-loaded Ag/polymeric NCs at very low doses of DOX on MCF-7 cells.

- ElBaz, M. N., Ziko, L., Siam, R., Mamdouh,\* W. (2016). Core-Shell Silver/Polymeric Nanoparticles-Based Combinatorial Therapy against Breast Cancer In-vitro. Scientific Reports (Nature Publishing Group), 6, (30729), 1-9.
- Nourihan S. Farrag, Hanan A. El-Sabagh, Abdulaziz M. Al-mahallawi, Abeer M. Amin, Ahmed AbdEl-Bary, Wael Mamdouh.\* Comparative Study on Radiolabeling and Biodistribution of Core-Shell Silver/Polymeric Nanoparticles-Based Theranostics for Tumor Targeting. *International Journal of Pharmaceutics*, 2017, 529, 123-133

## 1,8-Cineole-loaded Chitosan Nanoparticles: Optimization via Box-Behnken Design, Characterization, Release Kinetics, and Dual *In Vitro–In Silico* Evaluation Against HeLa Cancer Cell Line

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#### Abstract:

Cervical cancer remains a major global health challenge, necessitating the development of innovative drug delivery systems to enhance therapeutic outcomes. This study focuses on the formulation and evaluation of 1,8-cineole-loaded chitosan nanoparticles (CS-CIN NPs) for their anticancer efficacy against HeLa cervical cancer cells. Using Box-Behnken Design (BBD), the nanoparticles were optimized and synthesized via ionic gelation, resulting in a particle size of 249.6 nm, zeta potential of 22.2 mV, and high encapsulation efficiency. In vitro release studies pH-sensitive demonstrated release, with accelerated drug release in acidic environments (tumor-like conditions) and sustained release under physiological pH, ensuring prolonged drug availability. Cytotoxicity assays revealed a significant reduction in IC50 values for CS-CIN NPs compared to free 1,8-cineole, highlighting enhanced anticancer activity due to improved bioavailability and controlled drug release. In silico molecular docking studies confirmed strong binding affinities of 1,8-cineole to key particularly HeLa-associated targets, Topoisomerase II, suggesting mechanisms related to DNA replication inhibition and metastasis suppression. These findings demonstrate that CS-CIN NPs serve as an effective nanocarrier system for cervical cancer treatment, offering controlled drug release, improved cellular uptake, and potent anticancer activity against HeLa cells.

**Keywords**: Chitosan; 1,8 cineole; Nanoparticles; HeLa cell line; Box-Behnken



**Figure 1**: Figure 1. Contour plots illustrating the response surface analysis of various formulation parameters: (a) Zeta potential (mV), (b) Particle size (nm), (c) PDI (polydispersity index), (d) Loading Capacity (%), (e) Encapsulation Efficiency (%), and (f) Thermodynamic Stability (°C), as functions of 1,8 cineole concentration (%) and Surfactant concentration (%).

- 1. Shetta A, Kegere J, Mamdouh W. study encapsulated Comparative of peppermint and green tea essential oils in chitosan nanoparticles: Encapsulation, thermal stability, in-vitro release, antioxidant and antibacterial activities. Int J Biol Macromol. 2019 Apr 1;126:731-42.
- A. Attallah O, Shetta A, Elshishiny F, Mamdouh W. Essential oil loaded pectin/chitosan nanoparticles preparation and optimization via Box–Behnken design against MCF-7 breast cancer cell lines. RSC Adv. 2020;10(15):8703–8.

## Surface-Modified Drug Nanoparticles in Reinforced Hydrogel Matrix: A Sustainable Approach for Diabetic Wound Management

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#### Abstract:

Diabetic chronic wounds remain a significant clinical challenge due to impaired angiogenesis, epithelialization, and neutrophil function.<sup>1-2</sup> This study presents an innovative composite hydrogel system incorporating anti-inflammatory and local anesthetic drug nanoparticles (DNPs) within a biocompatible hydrogel matrix featuring a well-defined pore structure (Figure 1). The system targets both COX-2 and TNF-α pathways to reduce PGE2 secretion at wound sites. We utilize a reprecipitation method to prepare DNPs and modify the surface with phospholipidacrylate polymers, making them crosslinkable with PEGDA to significantly reinforce the hydrogel's porous structure. This enhancement enables optimal drug loading and sustained delivery, with our system achieving over 90% drug release efficiency and an adjustable therapeutic duration ranging from 4 to 72 hours. The composite hydrogel consists of crosslinkable DNPs, UV-induced crosslinked PEGDA, and porous component PEG, with carefully optimized fractions for ideal release properties. In vivo experiments demonstrate that the Gel-DNPs-AC system, through sustained antiinflammatory and analgesic effects, effectively promotes rapid transition of diabetic wounds from inflammatory to proliferative phase, enhancing keratinocyte survival and migration facilitating neovascularization while and collagen alignment. Compared to untreated controls, this hydrogel accelerates healing rates by an impressive 17-fold. Beyond diabetic wounds, this platform shows potential for postsurgical applications, with its designable shape allowing versatile use on wound as a drug reservoir.



Figure 1: Scheme of DNPs and nanodrugshydrogel composite preparation.



**Figure 4**: a) Schematic illustration of the design of animal experiments to test the therapeutic effect of composite hydrogel in the normal and diabetic mouse model. b) Representative images of the wounds for 14 days. c) Illustration of wound size at different time points, normalized to day 0. d) Qualification of wound size change during 14 days of post wounding.

**Keywords**: wound healing, composite hydrogels, nanoparticle drugs, antiinflammation, synergy therapy, biomedical applications.

- 1. Watkins, D. A., Ali, M. K. (2023) Measuring the global burden of diabetes: implications for health policy, practice, and research, *The Lancet*, 402(10397), 163-165.
- Qi, X., Cai, E., Xiang, Y., Zhang, C., Ge, X., Wang, J., ... & Shen, J. (2023) An Immunomodulatory Hydrogel by Hyperthermia-Assisted Self-Cascade Glucose Depletion and ROS Scavenging for Diabetic Foot Ulcer Wound Therapeutics, *Advanced Materials*, 35(48), 2306632.

## **Posters Sessions Abstracts**

## Morphological and Structural Engineering of Niobium Selenide Nanostructures via Chemical Vapor Transport

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#### Abstract:

Two-dimensional (2D) van der Waals (vdW) layered transition metal dichalcogenides (TMDs), have garnered considerable attention owing to their intriguing physical and chemical properties. in particular are fascinating Metallic TMDs materials due to their special characteristics such as Weyl semimetals<sup>1</sup>, charge density waves<sup>2</sup> and superconductivity<sup>3</sup>. Recently, interest in 2D vdW materials has expanded to encompass onedimensional (1D) vdW structures, whereas 1D vdW materials are mainly nanostructures, such as ribbons, wires, and molecular chains. <sup>4</sup>They have wide practical applications in transistors<sup>5</sup>, photodetectors<sup>6</sup>, thermoelectric devices<sup>7</sup>, solar cells<sup>8</sup>, and water splitting. <sup>9</sup>The field of study is undergoing continuous expansion, with previously less researched materials are now being studied. One of these materials is niobium selenide. There are several stoichiometric compounds in the system Nb-Se, such as NbSe<sub>2</sub>, Nb<sub>2</sub>Se<sub>9</sub> and both crystallize in a layered structure. In this study, the effect of the growth parameters on the morphological, structural and electrical transport properties of niobium selenide nanostructures using the bottom-up chemical vapor transport (CVT) method was explored. Thermodynamic calculations were performed to optimize the growth process, the transport agent was varied from I2 to NbCl5 resulted in the formation of high quality of NbSe<sub>2</sub> nanocrystals and Nb<sub>2</sub>Se<sub>9</sub> nanowires respectively. While changing the growth temperature leads to formation of NbSe<sub>2</sub> at (T1 = 1000 °C, T2 = 800 °C)and  $(NbSe_4)_3I$  at (T1 = 600 °C, T2 = 400 °C). The effect of controlling the amount of transport agent and the thermal oxidation duration of the substrate on the morphology and the growth mode were also investigated here. The chemical composition and morphology of the nanocrystals were analyzed by energy dispersive X-ray spectroscopy, scanning electron microscopy, atomic force microscopy and Raman spectroscopy. The high crystalline quality were confirmed by high-resolution transmission

electron microscopy and electrical properties were invisigated by magneto-transport measuremnts. This study opens the path for the study of further interesting materials based on intercalated or doped NbSe<sub>2</sub>

**Keywords**: 2D vdW materials, 1D vdW materials, niobium selenide, nanostructutreschemical vapor transport, transport agent, morphological, transport measuremnts.



Figure 1: Optical-microscopy images of 2H-NbSe<sub>2</sub> nanocrystals deposited on C-plane sapphire (0001) substrates.

- 1. S. Jia, S.-Y. Xu and M. Z. Hasan, *Nature materials*, 2016, 15, 1140-1144.
- Y. S. Hor, Z. Xiao, U. Welp, Y. Ito, J. Mitchell, R. Cook, W. Kwok and G. W. Crabtree, *Nano letters*, 2005, 5, 397-401.
- 3. Y. S. Hor, U. Welp, Y. Ito, Z. Xiao, U. Patel, J. Mitchell, W. Kwok and G. W. Crabtree, *Applied Physics Letters*, 2005, 87, 142506.
- 4. D. L. M. Cordova, K. Chua, R. M. Huynh, T. Aoki and M. Q. Arguilla, *Journal of the American Chemical Society*, 2023, 145, 22413-22424.
- O. Island, A. J. Molina-Mendoza, M. Barawi, R. Biele, E. Flores, J. M. Clamagirand, J. R. Ares, C. Sánchez, H. S. Van Der Zant and R. D'Agosta, 2D Materials, 2017, 4, 022003.

- J.-J. Tao, J. Jiang, S.-N. Zhao, Y. Zhang, X.-X. Li, X. Fang, P. Wang, W. Hu, Y. H. Lee and H.-L. Lu, ACS nano, 2021, 15, 3241-3250.
- D.-Y. Chung, T. P. Hogan, M. Rocci-Lane, P. Brazis, J. R. Ireland, C. R. Kannewurf, M. Bastea, C. Uher and M. G. Kanatzidis, *Journal* of the American Chemical Society, 2004, 126, 6414-6428.
- Y. Zhou, L. Wang, S. Chen, S. Qin, X. Liu, J. Chen, D.-J. Xue, M. Luo, Y. Cao and Y. Cheng, *Nature Photonics*, 2015, 9, 409-415.
- 9. W. Yang, J. Ahn, Y. Oh, J. Tan, H. Lee, J. Park, H. C. Kwon, J. Kim, W. Jo and J. Kim, *Advanced Energy Materials*, 2018, 8, 1870061.

# Fluorescent half-salen phenoxy-imine zinc complexes to reveal exogenous and endogenous H<sub>2</sub>S

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#### Abstract:

For hundred of years H<sub>2</sub>S has been solely known as a toxic gas, causing life destructions and extinctions on the earth. The revolutionary discovery that this molecule is endogenously produced in mammalian tissues and exherts physiological and/or pathophysiological functions within human body, depending on its body concentration motivates its entrance in the family of the 'so-called' gasotransmitters (together with NO and CO).[1,2] In this context an upsurge of model systems and investigative tools of how H<sub>2</sub>S and related Reactive Sulfur Species (RSS) participate in complex biological processes were devised. In particular, fluorescent probes for H<sub>2</sub>S detection have been proven as important tools for investigating the composite roles of this molecule in complex biological systems. A new common approach aiming at developing such tools makes use of "activitybased probes" which pair a H<sub>2</sub>S-mediated chemical reaction to a fluorescence response. In this contribution, the synthesis and the reactivity with HS<sup>-</sup> of a family of half-salen Zn complexes will be reported. We provide evidence that HS<sup>-</sup> binds the zinc center of all the complexes under investigation. Interaction with HS<sup>-</sup> results in its coordination to the Zn center for all the complexes under investigation. Bio-imaging experiments indicate the potential in using this class of compounds for the detection of H<sub>2</sub>S in living cells.[3] (Figure 1)

**Keywords**: Nanosensor, fluorescent probe, H<sub>2</sub>S, cell culture, metal complexes, biomedical applications.



**Figure 1**: Figure illustrating the capability of the metal complex to recognize the H<sub>2</sub>S production in living cells through the fluorescent adduct.

- 1. Li L., et al., (2007) An overview of the biological significance of endogenous gases: new roles for old molecules, *Biochem Soc Trans*, 35 (5): 1138–1141.
- 2. Li L., et al., (2008) Putative biological roles of hydrogen sulfide in health and disease: a breath of not so fresh air? *Trends pharmacol Sci*, 29(2):84-90.
- 3. Trerotola A., et al., (2025) Fluorescent halfsalen phenoxy-imine zinc complexes to reveal exogenous and endogenous H<sub>2</sub>S, *Journal of Inorganic Biochemistry*, 267: 112875.

## Very High Efficacy *In Vitro* Terapy of Human Melanoma Cancer by Superparamagnetic Hyperthermia with Magnetite-Hydroxypropyl-Gamma-Cyclodextrin Nanoparticles

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#### Abstract:

In this paper we show new results on obtaining very high efficacy (up to 98%), and without toxicity [1], in the alternative therapy of human melanoma cancer (A375 cancer cells) in vitro by hyperthermia superparamagnetic using biocompatible magnetite-hydroxypropylgamma-cyclodextrins nanoparticles previously obtained by us [2]. Magnetic magnetite nanoparticles (Fe<sub>3</sub>O<sub>4</sub>) have a mean diameter of ~15.8 nm and have been used in therapy for the concentrations of 1, 5 and 10 mg/mL in cell suspension. The therapy was performed for 30 min. at a temperature of 43 °C obtained by applying an alternating magnetic field with a frequency of 312.4 kHz and the amplitudes of 168, 208, 370 Gs as a function of the concentration of nanoparticles. Our results show a significant increase in efficacy in destroying A375 melanoma cancer cells, up to 98%, compared to previous results on squamous skin carcinoma, where the maximum percentage obtained was 83% [3]. This suggests that melanoma cancer cells are much more sensitive to magnetic hyperthermia under the conditions we established than squamous skin carcinoma cells. Also, the result confirms the viability of superparamagnetic hyperthermia as an alternative cancer therapy using magnetite nanoparticles decorated with hydroxypropylgamma-cyclodextrins, under the conditions previously established by us [2,3], and paves the way for the application of this therapy in vivo and then in clinical trials.

**Keywords**: *in vitro* superparamagnetic hyperthermia, alternative cancer therapy, human melanoma cancer, biocompatible magnetite-

#### hydroxypropyl-gamma-cyclodextrins nanoparticles. **References:**

- ISO 10993-5:2009, Biological evaluation of medical devices–Part 5: Tests for in vitro cytotoxicity. ISO Catalogue, Edition 3. International Standard Organization: Geneva, Switzerland. Available online: https://www.iso.org/standard/36406.html
- Caizer, C., Caizer, I.S., Racoviceanu, R., Watz, C.G., Mioc, M., Dehelean, C.A., Bratu, T., Soica, C. (2022) Fe<sub>3</sub>O<sub>4</sub>-PAA– (HP-γ-CDs) biocompatible ferrimagnetic nanoparticles for increasing the efficacy in superparamagnetic hyperthermia, *Nanomaterials*, 12, 2577.
- Caizer-Gaitan, I.S., Watz, C.G., Caizer, C., Dehelean, C.A. Bratu, T., Crainiceanu, Z., Coroaba, A., Pinteala, M., Soica, C.M. (2024) In vitro superparamagnetic hyperthermia employing magnetite gammacyclodextrin nanobioconjugates for human squamous skin carcinoma therapy, *Int. J. Molec. Sci.*, 25, 8380.
## "Targeted Doxorubicin delivery and release within breast cancer environment using PEGylated chitosan nanoparticles labeled with monoclonal antibodies"

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#### Abstract

The potential of nanobiomedical field for developing a promising therapeutic nano-sized drug delivery system is seen to be a great pharmaceutical trend for encapsulation and release of various antineoplastic drugs. In this context, the current work is targeting preparation of biodegradable chitosan nanoparticles (CSNP) that have been intended for selective and sustained release of doxorubicin (DOX) within breast tumor microenvironment. Surface modification of these CSNP with Polyethylene glycol (PEG) was performed in order for enhancing its blood circulation time without being opsonized or captured by immunogenic reticuloendothelial system (RES). PEG has maintained high particles stability profile, and enhanced its surface positive charge for the sake of intracellular attachment via electrostatic attachment with negatively charged tumor cell membrane. Advanced tumor selectivity has been achieved through functionalization of two different types of breast cancer specific monoclonal antibodies (mAb); anti-human mammaglobin (Anti-hMAM) and anti-human epidermal growth factor (Anti-HER2) in two different separate nano formulations. This functionalization has the potential of evading

systemic side effects of parenteral free DOX and promoting cancerous endocytosis through mediated interaction. receptor In-vitro cytotoxicity effects of PEGylated DOX loaded CSNP, free DOX, Anti-HER2 PEGylated DOX loaded CSNP and Anti-hMAM PEGylated DOX loaded CSNP were tested against breast cancer cell line (MCF7) and normal fibroblast cell line (L929). Notably, Anti-hMAM PEGylated DOX loaded CSNP and Anti-HER2 PEGylated DOX loaded CSNP formulations were the most cytotoxic against MCF7 cancer cells than L929 normal cells compared to free DOX. Confirmatory bright filed images of the two cell lines have exhibited cancerous cellular damage after 24 hours exposure time to these nano formulations. Finally, we believe that dose dependent system toxicity of freely ingested DOX can be hindered with such targeted nano formulated drug delivery system.

**Key words:** PEGylated chitosan nanoparticles. monoclonal antibody, mAb, Anti-HER2, AntihMAM, surface functionalized, nano formulation, targeted drug delivery, MCF7, L929, doxorubicin, chitosan, PEG, selective anti-cancer, systemic, breast tumor, cancer, chemotherapeutic agent.



Figure 1: Graphical diagram of DOX encapsulation and release within tumor cell

- Le, W.; Chen, B.; Cui, Z.; Liu, Z.; Shi, D. Detection of Cancer Cells Based on Glycolytic-Regulated Surface Electrical Charges. *Biophys Rep* 2019, 5 (1), 10–18. <u>https://doi.org/10.1007/s41048-018-0080-0</u>.
- Ayoub, N. M.; Al-Shami, K. M.; Yaghan, R. J. Immunotherapy for HER2-Positive Breast Cancer: Recent Advances and Combination Therapeutic Approaches. *Breast Cancer (Dove Med Press)* 2019, *11*, 53–69. <u>https://doi.org/10.2147/BCTT.S175360</u>.

# Inhibitory effect on retinal neovascularization of gold nanodisks optically tuned for optical coherence tomography

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#### Abstract:

Bare gold nanospheres have been shown to have anti-angiogenic effects but are optically unfavorable because their resonant wavelength lies in the visible spectrum. Here, we design gold nanodisks with a higher scattering capability than gold nanorods and with a resonant wavelength at near-infrared region- the area where the source of light utilized by optical coherence tomography (OCT) lies. With a physical synthesis system, we then fabricate 160-nm-sized gold nanodisks exhibiting resonant wavelength at 830 nm. The synthesized nanoparticles were successfully visualized in in vivo OCT at concentrations as low as 1 pM. After demonstrating their binding ability to vascular endothelial growth factor (VEGF), we show that they suppress VEGFinduced migration of endothelial cells. Finally, we demonstrate that intravitreally injected gold nanodisks attenuate neovascularization of oxygen-induced retinopathy in mice, in a dose dependent manner, such that they are cleared from the vitreous within 2 weeks without histologic or electrophysiologic toxicity

**Keywords**: Gold nanodisk; Near-infrared; Optical coherence tomography; Intraocular application; Angiogenesis inhibitor; Retinal neovascularization



**Figure 1**: Gold nanodisks have higher scattering efficiencies and resonant wavelength can be modulated by changing size. Negative zeta potential of bare gold facilitates diffusion in the vitreous. As a result, 160-nm-sized bare gold nanodisks exhibiting resonant wavelength at 830

nm where the source of light utilized by OCT lies were fabricated. Intravitreally injected gold nanodisks showed strong signal intensity in *in vivo* OCT and could attenuate retinal neovascularization of oxygen-induced retinopathy mice.

#### **References:**

 Song HB, Wi JS, Jo DH, Kim JH, Lee SW, Lee TG, Kim JH (2017) Nanoparticleprotein complexes mimicking corona formation in ocular environment, *Nanomedicine*, 13(6), 1901-1911

# A measurement method for assessing the dimensions of shape patterns utilizing silver-nano inks in printed electronics

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## Abstract:

This study introduces an advanced algorithm for accurately measuring the geometry and printability of shape patterns, which are crucial in nanoparticle-based printed electronic devices. While many studies have investigated printability, few have established international standards for measuring the dimensions and printability of shape patterns. The proposed algorithm aims to lay the foundation for such standards.

The algorithm incorporates three core concepts: extraction of edges of printed patterns and identification of pixel positions, identification of reference edges via the best-fitting of the shape pattern, and calculation of different pixel positions of edges related to reference edges. This method allows for the measurement of pattern geometry and printability, including edge waviness and widening, by considering all pixels comprising the edges.

The study details the measurement methods for both rectangle and circle patterns. For rectangles, vertical and horizontal reference lines are used to calculate width, height, and center, and widening is determined by comparing with the original design. Edge waviness is evaluated using the average and standard deviation of the pixel distances from the centerlines. For circles, the identified using center is intersecting perpendicular bisectors of lines drawn across the edge. The mean radius, standard deviation, and widening are then calculated based on the distance of each edge pixel from the center compared to the original design radius. Experimental verification using roll-to-roll direct gravure printing of milliscale rectangle and circle patterns demonstrated the algorithm's accuracy.

The study concludes that the proposed algorithm reliably quantifies the geometry and quality of printed patterns. This has potential applications in real-time pattern quality evaluation, process optimization using statistical or AI-based methods, and the establishment of International Electrotechnical Commission (IEC) standards for shape patterns. The algorithm can also be applied to complex and irregular patterns by combining the methods for rectangles and circles or by aligning printed patterns with their designs

**Keywords**: printed electronics, printing, geometry, printability, quantification.



Figure 1: Pattern quantification algorithm



**Figure 2**: Quantification of the pattern geometry using the processed images

- 1. Lee, J., Kim, C.H. (2023) Advanced Algorithm for Reliable Quantification of the Geometry and Printability of Printed Patterns, *Nanomaterials*, 13, 1597.
- Lee, J.; Shin, K.; Jung, H. (2022) Control scheme for rapidly responding register controller using response acceleration input in industrial roll-to-roll manufacturing systems. IEEE Trans. Ind. Elect. 69, 5214– 5224.

# Poly(butylene succinate) (PBS) films composites with carbon black

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#### Abstract:

The growing environmental impact of conventional plastics has intensified the global ecological crisis, encouraging the development of sustainable and biodegradable alternatives. Biodegradable polymers and their composites reinforced with renewable fillers have attracted considerable scientific attention due to their environmental benefits and their potential to mitigate plastic pollution [1].

Among different biodegradable polymers, Poly (butylene succinate) (PBS) is an arousing a lot of interests thanks to its biodegradability, melt processability, thermal resistance and melt processability, making it a promising material for applications in the fields of environmental protection and human health preservation.

However, PBS has limitations associated with its thermal stability, high flammability and relatively poor mechanical properties. To overcome these disadvantages a filler, such as carbon black (CB), can be used as a reinforcing filler. CB can enhance the mechanical properties of polymer composite, such as tensile strength and elastic modulus, when used as a filler. The incorporation of a small amount of CB into biodegradable polymer matrices can improve physical performance and expand the functional applicability of biodegradable polymers in advanced engineering and environmental applications [2]. Moreover, carbon black (CB) exhibits excellent electrical conductivity [3] its incorporation in the polymer matrix is expected to modify electrical properties of the obtained composite. In particular, it is expected that the material changes its electrical behavior from a typical insulator to those of a conductive once as the filler content increases. In order to explore this characteristic, films of PBS were prepared by solution casting, filled with a different amount of CB, and characterized in terms of electrical conductivity as function of the filler content. It has been obtained that a concentration of only 1% weight in filler amount leads to double the electrical conductivity of the pristine matrix.

**Keywords**: biodegradable polymer, carbon material, composite, electrical conductivity, electrical properties.

#### **References:**

- 1. Ojijo, V., Ray, S. S., (2013). Processing strategies in bionanocomposites, *Prog. Polym. Sci.*, 38, 1543-1589.
- Ge, F., Wang, X., Ran, X. (2017). Properties of biodegradable poly (butylene succinate) (PBS) composites with carbon black. *Polym. Sci., Series A*, 59, 416-424.
- Chen, Z., Hu, J., Ju, J., & Kuang, T. (2019). Fabrication of poly (butylene succinate)/carbon black nanocomposite foams with good electrical conductivity and high strength by a supercritical CO<sub>2</sub> foaming process. *Polymers*, 11, 1852.

### Acknowledgements:

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# CuO Nanoparticles-Decorated Femtosecond Laser-Irradiated WS<sub>2</sub>– WO<sub>3</sub> Heterojunctions to Realize Selective H<sub>2</sub>S Gas Sensors

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#### Abstract:

Femtosecond (FS) laser irradiation is an easy and highly effective strategy for enhancing the sensing properties of resistive gas sensors. In this study, we applied this technique to WS<sub>2</sub> nanosheets (NSs) to generate WS<sub>2</sub>-WO<sub>3</sub> Subsequently, heterojunctions. they were decorated with CuO nanoparticles (NPs). Different characterization techniques demonstrated the formation of CuO-decorated WS<sub>2</sub>–WO<sub>3</sub> heterojunction NSs with the desired morphology, phase, and chemical composition. Based on H<sub>2</sub>S gas-sensing studies, while nonirradiated WS<sub>2</sub> sensors exhibited poor sensing performance, a combination of FS laser irradiation and CuO decoration led to significant performance improvement for H<sub>2</sub>S sensing in terms of response and selectivity (Figure 1). Enhanced performance is related to the formation of plenty of WS<sub>2</sub>–WO<sub>3</sub> heterojunctions, oxygen vacancies, and the conversion of CuO to CuS with high metallic conductivity (Figure 2). We believe that the strategy used in this work can pave the way for the realization of lowtemperature, sensitive, and selective H<sub>2</sub>S gas sensors.

Keywords:  $WS_2$  Nanosheets, Femtosecond laser irradiation, CuO–decoration,  $H_2S$  gas sensor, Sensing mechanism.



Figure 1: Dynamic resistance curves of (a) FS laser-irradiated  $WS_2$ – $WO_3$  NS gas sensor and (b) CuO-decorated FS laser-irradiated  $WS_2$ – $WO_3$ NS gas sensor to 10 ppm of various gases at 20 °C and 1 V of applied voltage. (c) Selectivity histograms of different gas sensors to 10 ppm of various gases at 20 °C.



**Figure 2**: Energy band levels of  $WS_2$  and  $WO_3$ (a) before and (b) after contact; (c) band bending of CuO and  $WO_3$  in intimate contact in (c) air; and (d) subsequent exposure to  $H_2S$ .

- Kim, J.-H., Mirzaei, A., Kim, H.W., Kim, S.S. (2019), Realization of Au-decorated WS<sub>2</sub> nanosheets as low power-consumption and selective gas sensors, *Sens. Actuators B*, 296, 126659.
- Zanolli, Z., Leghrib, R., Felten, A., Pireaux, J.-J., Llobet, E., Charlier, J.-C. (2011), Gas sensing with Au-decorated carbon nanotubes, *ACS Nano*, 5, 4592–4599.

## Comprehensive Kinetic Modeling and DFT Analysis of Cationic and Anionic Dye Photocatalytic Degradation: Insights for Green Chemistry and Water Treatment Technologies

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### Abstract:

Industrial dyes such as cationic rhodamine B (RhB) and anionic bromocresol green (BCG) are widely used in textiles, food processing, pharmaceuticals, and research applications. Despite their utility, their release into water bodies poses serious environmental concerns due to their high stability, persistence, and resistance to natural degradation. These dyes can significantly reduce light penetration in aquatic ecosystems, disrupt photosynthesis, and harm aquatic life, highlighting the urgent need for efficient water treatment strategies. Among various remediation methods, photocatalytic degradation has emerged as a promising solution due to its ability to completely mineralize organic pollutants<sup>1</sup>.

This study investigates the photocatalytic degradation of RhB and BCG using oxygenvacancy-enriched ZnO as a catalyst, focusing on how dye charge and molecular structure influence degradation mechanisms. The catalyst was modified by hydrogen reduction (10% H<sub>2</sub>/Ar at 500°C) to introduce oxygen vacancies, confirmed through comprehensive material characterization <sup>2</sup>. A kinetic model was developed to simultaneously describe adsorption and degradation, incorporating pH-dependent dye speciation based on pK<sub>a</sub> values <sup>3</sup>.

The findings in this work indicate that degradation predominantly occurs on the catalyst surface under acidic conditions, while at basic pH, hydroxyl radicals in solution drive the process. Density functional theory (DFT) calculations further elucidate these trends, revealing shifts in electrostatic potential that influence dye interactions with reactive species (Figure 1)<sup>4</sup>. These insights provide a mechanistic of understanding charge-dependent photocatalytic behavior, offering guidance for optimizing ZnO-based photocatalysts for wastewater treatment applications.

**Keywords**: Photocatalysis, Kinetic modeling, DFT calculations, ESP maping, Cationic and anionic dyes, Oxygen vacancies.



**Figure 1**: Simulations of a) photocatalytic degradation of RhB in the solution and b) photocatalytic degradation of RhB on the surface of the catalyst. c) Electrostatic potential (ESP) of neutral RhB, d) ESP of protonated RhB.

- Ranjbari, A., ..., Heynderickx, P. M. (2025). Comparative photocatalytic degradation of cationic rhodamine B and anionic bromocresol green using reduced ZnO: A detailed kinetic modeling approach. *Chemosphere*, 371, 144052.
- Ranjbari, A., ..., Heynderickx, P. M. (2023). Oxygen vacancy modification of commercial ZnO by hydrogen reduction for the removal of thiabendazole: Characterization and kinetic study. *Applied Catalysis B: Environmental*, 324, 122265.
- Ranjbari, A., ..., Heynderickx, P. M. (2022). Novel kinetic modeling of thiabendazole removal by adsorption and photocatalysis on porous organic polymers: Effect of pH and visible light intensity. *Chemical Engineering Journal*, 431, 133349.
- Ranjbari, A.,, Heynderickx, P. M. (2025). The adsorption/photocatalytic degradation kinetics of oxygen vacancy-enriched ZnO in relation to surface functional groups of cationic/anionic dyes. *Chemical Engineering Journal*, 505, 159526.

# Evaluating the Catalytic Performance of Mo<sub>3</sub>P for the Hydrogen Evolution Reaction in Alkaline Media

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#### Abstract:

Catalysis plays a crucial role in many sectors, contributing to more than one third of the global gross domestic product. In light of the net-zero greenhouse gas emissions objective, catalysis is becoming increasingly significant in the energy sector. Considerable attention is being paid to cost-effective developing and efficient electrocatalysts for water electrolysis, which would enhance the performance of water electrolysers and thus promote the adoption of this technology for energy storage and cleaner hydrogen production. The catalytic potential of various materials, ranging from those with lownoble metal content to transition metal-based catalysts, has been explored. The present work investigates the electrocatylytic activity of trimolybdenum phosphide (Mo<sub>3</sub>P) for the hydrogen evolution reaction (HER) in alkaline environment, as well as the mechanism of this reaction. Mo<sub>3</sub>P was synthesized using the citrate sol-gel method, followed by two-step sintering process - first in air and then in a reducing atmosphere. Its electrocatalytic activity for HER was evaluated by linear sweep voltammetry (LSV) using a stationary glassy carbon electrode (S-GCE) with a disk diameter of 3 mm. A total of 0.3 mg of catalyst was loaded onto the S-GCE. As shown in the LSV curve reported with 90 % iR compensation (Figure 1), Mo<sub>3</sub>P exhibited relatively high electrocatalytic performance, requiring only 272 mV to achieve a current density of 10 mA.cm<sup>-2</sup>. In addition to its activity, the HER mechanism on this catalyst was also investigated. Reaction mechanism, specifically rate-determinig step of HER on studied catalyst, was assumed from Tafel slope derived from LSV curve. The Tafel slope of 100 mV.dec<sup>-1</sup> (Figure 1, inset) suggests that hydrogen adsorption on the catalyst surface is the rate-determining step.

**Keywords**: catalysis, hydrogen evolution reaction, transition metal phosphide, water electrolysis.



**Figure 1**: HER LSV curve and Tafel slope (inset) of trimolybdenum phosphide in alkaline environment.

- Gu, J., Zhu, Y., Zheng, H., Sun, C., Su, Z. (2024) Small-sized Ni-Co/Mo<sub>2</sub>C/Co<sub>6</sub>Mo<sub>6</sub>C<sub>2</sub>@C for efficient alkaline and acidic hydrogen evolution reaction by an anchoring calcination strategy, *Front. Chem. Sci. Eng.*, 18.
- 2. Raveendran, A., Chandran, M., Dhanusuraman, R. (2023) A comprehensive review on the electrochemical parameters and recent material development of electrochemical water splitting electrocatalysts, *RSC Adv.*, 13, 3843-3876.
- Salonen, L. M., Petrovykh, D. Y., Kolen'ko, Y. V. (2021) Sustainable catalysts for water electrolysis: Selected strategies for reduction and replacement of platinum-group metals, *Mater. Today Sustain.*, 11-12.
- Taseska, T., Yu, W., Wilsey, M. K., Cox, C. P., Meng, Z., Ngarnim, S. S., Müller, A. M. (2023) Analysis of the Scale of Global Human Needs and Opportunities for Sustainable Catalytic Technologies, *Top. Catal.*, 66, 338-374.

# Carrageenan as an Ecological Binder for Sulfur-Based Nanostructured Electrodes for Li-S batteries

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#### Abstract:

Carrageenan, a natural polysaccharide derived from red seaweed, has emerged as a promising ecological binder for lithium-sulfur (Li-S) batteries. Its abundant functional groups enable strong adhesion with sulfur cathodes while mechanical integrity and enhancing the electrochemical stability of the electrode. Unlike conventional synthetic binders, carrageenan offers sustainability, biodegradability, and improved electrolyte compatibility, reducing polysulfide dissolution and improving cycling performance (1,2). This study explores the structural advantages of carrageenan-based binders and their impact on Li-S battery efficiency, highlighting their potential as a green alternative for next-generation energy storage systems. Sulfur based nanostructured electrodes using carrageenan were fabricated without the toxic solvent N-methyl-2-pyrrolidone (NMP), relying solely on water as a solvent and dispersant, making the process both scalable and cost-effective. Our study demonstrated exceptional capacity retention of 69.1% at 4 C after 1000 charge-discharge cycles with carrageenan-based electrodes, compared to 39.3% retention at 4 C after 500 cycles for PVDF-based electrodes.



**Figure 1:** Electrochemical performance a) Changes in specific discharge capacity of PVDF10 and CARR10 at different C rates, b) Specific discharge capacities of PVDF10 and CARR10 at 0.1 C rates for 250 cycles with the corresponding CE values, c) Cyclic performance of the different carrageenan-containing cells obtained at 0.1 C rate, d) Cyclic performance of

the different carrageenan-containing cells obtained at 4 C rate.

Galvanostatic charge-discharge measurements (Fig. 1) demonstrated that cells containing 10 wt% carrageenan exhibited superior performance compared to those with an equivalent amount of PVDF, achieving higher specific discharge capacity, improved sulfur utilization, and enhanced long-term cyclability. Scanning Electron Microscopy-Focused Ion Beam (SEM-FIB) analyses conducted before and after cycling revealed reduced electrode fracturing with increased carrageenan content. Elemental mapping of the cathodes showed a more uniform sulfur distribution and identified sodium and potassium near sulfur deposits, suggesting that carrageenan effectively coats the sulfur particles.

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**Keywords**: batteries, binders, Li-S, energy storage, nanostructured surfaces, capacity fading, long-life storage systems.

- B. Chang, et al., Carrageenan as a sacrificial binder for 5 V LiNi0.5 Mn1.5O4 cathodes in lithium-ion batteries, Adv. Mater. 35 (2023), https://doi.org/ 10.1002/adma.202303787 e2303787
- D. Zalka, A. Vizintin, A. Maximenko, Z. Pászti, Z. Dankházi, K. Hegedüs, L.S. Shankar, R. Kun, K. Saksl, A. Straková Fedorková, P. Jóvári, "Improving lithiumsulfur battery performance using a polysaccharide binder derived from red algae", *Comm. Mat.*, 6 (1), art. no. 17, 2025, DOI: 10.1038/s43246-025-00734-1

# Effect of acid etching on the supercapacitive performance of electroless Ni-B coatings

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## Abstract:

Ni-B coatings deposited by electroless method are well-known for their excellent mechanical properties e.g. high hardness and wear resistance, that allow them to be widely used in different industrial fields [1,2]. Furthermore, they also possess pseudocapacitive properties, which makes them suitable for use in supercapacitor applications as well [3]. The surface morphology, crystalline structure and B-content basically affect the electrochemical properties of the coatings [4]. It is also known, that the presence of porosity can significantly increase the specific capacitance of the electrode materials. In our study, we report on a facile, easy-to-implement method to introduce a porous structure into the Ni-B coated copper sheet electrodes by acid etching in HNO<sub>3</sub>, where the coating serves as an active electrode material. This method can be used to increase the specific surface area of the coatings. and improve the overall electrochemical performance. Our study focuses on the investigation of the effect of etching time on the physical properties, micro-and phase structure as well as the electrochemical properties of the Ni-B coatings. The electrochemical performance was evaluated by cyclic voltammetry (CV), galvanostatic chargedischarge (GCD) and electrochemical impedance spectroscopy (EIS). By increasing the etching time, the porosity (number, size and shape of pores) can be tailored to achieve an optimal porenetwork for the Faradaic reactions to take place at the electrode/electrolyte interface. In alkaline KOH electrolyte, the reversible transformation of  $Ni^{2+} \leftrightarrow Ni^{3+}$  can be exploited by oxidationreactions. resulting reduction in pseudocapacitance that can be used as energy storage mechanism.

**Keywords**: supercapacitance, pseudocapacitor, electroless deposition, Ni-B coating, chemical etching, porous structure



**Figure 1**: Microstructure of (a) as-deposited Ni-B coating, (b) Ni-B coating etched for 15 s in 7M HNO<sub>3</sub>, c) Cyclic voltammetry (CV) results of the coatings, A<sub>electrode</sub>: 5.02 cm<sup>2</sup>, v: 10 mV/s

- V. Niksefat, F. Mahboubi, Tribological performance of plasma-nitrided selflubricant electroless Ni-B-graphite composite coatings, Tribology International 198 (2024) 109905.
- C. Chenna Raidu, S. Boominathasellarajan, N. Arunachalam, Tribological evaluation of ZrO2 and YSZ nanoparticle reinforced electroless Ni–B coatings, Ceramics International 50 (2024) 15461–15471.
- W. Li, S. Wang, M. Wu, X. Wang, Y. Long, X. Lou, Direct aqueous solution synthesis of an ultra-fine amorphous nickel–boron alloy with superior pseudocapacitive performance for advanced asymmetric supercapacitors, New J. Chem. 41 (2017) 7302–7311.
- M. Czagany, S. Hompoth, M. Windisch, P. Baumli, Investigation of the Supercapacitive Behavior of Electroless Ni-B Coatings, Metals 13 (2023) 1233.

## Interfacial behavior between the electrolyte and the electrode

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#### Abstract:

Understanding how electrolytes interact with (electrode) surfaces—specifically metal regarding wettability-is critically important across various industrial and chemical technology fields. This is especially true in contexts such as metal corrosion, electrochemical synthesis (where effective electrode-electrolyte contact is a crucial question) [1], and processes within the oil industry, like water-oil separation [2,3], among others. Numerous studies have examined the wettability in water-metal systems [4]; however, their findings often contradict each other, a point highlighted by Schrader [5].

White [6] attributes the difference in the wetting behavior to the forming of oxide films with uncertain composition and thickness during surface cleaning, which can lead to complete wetting. Conversely, in typical water-metal interfaces, the contact angle ( $\Theta$ ) is often around 60°, a value supported by Erb's experimental observations on noble metal surfaces [7].

A universal equation that accurately predicts either the wettability of metals by electrolytes or the adhesion energy in metal-electrolyte systems needs to be used.

The objective of our study is to measure the contact angles of both polar and non-polar liquids across a broad selection of metal surfaces and to establish a relationship between these contact angles and the intrinsic properties of the metal substrates based on our experimental data.

**Keywords**: electrodes, electrolytes, interfacial behavior, wettability

## **References:**

- 1. Wei J.Z.; Llle O.B. Influence of Wettability on Two- and Four-Electrode Resistivity Measurements on Berea Sandstone Plugs, SPE Form Eval 1991;6:470–476.
- Kang Z.; Wang S.; Fan L.; Xiao Z.; Wang R.; Sun D. Surface wettability switching of metal-organic framework mesh for oil-water separation, Mater Lett 2017;189:82–85.
- Zhu M.; Liu Y.; Chen M.; Xu Z.; Li L.; Zhou Y. Metal mesh-based special wettability materials for oil-water separation: A review

of the recent development, J Pet Sci Eng 2021;205:108889.

- 4. Trevoy D.J.; Johnson H. The Water Wettability of Metal Surfaces, J Phys Chem 1958;62:833–837.
- Schrader M.E. Wettability of clean metal surfaces, J. Colloid Interf Sci 1984;100:372– 380.
- 6. White M.L. The Wetting of Gold Surfaces by Water 1, J Phys Chem 1964;68:3083–3085.
- Erb R.A. Wettability of Metals under Continuous Condensing Conditions, J Phys Chem 1965;69:1306–1309

# The impact of copper anodization and microwave plasma treatment on energy storage applications

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#### Abstract:

The CuO/Cu2O nanowires were grown on copper by anodizing using a sodium hydroxide solution from 0 to 900s. After growth, the nanowires were heat treated at 400 °C for 1 h, the originality of this work is to improve surface activity by anodization of cupper substrate, followed by functionalization with nitrogen gas for 2 hours. By varying the anodizing time from 0 to 900s, changes in structure, morphological and electrochemical CuO/Cu2O properties were analysis observed. XRD confirmed the polycrystalline nature of CuO/Cu2O with a face cubic phase. SEM imaging showed significant changes in density and surface roughness. Super-Capacitive properties were evaluated using cyclic voltammetry, galvanostatic chargedischarge and chemical impedance spectroscopy (EIS) techniques, with Cu-600s-N2 having the highest specific capability of 1250 mF/cm2. Dunn's method was used to analyze the contribution of capacitive and diffusive mechanisms to charge storage. EIS results indicated excellent electron conductivity. The study suggests that Cu-600s-N2 promising applications for energy storage

**Keywords**: Copper, anodization, plasma micro wave, supercondensateurs, storage energy.



**Figure 1**: Figure illustrating the effectiveness of plasma in energy storage applications.

- A. Bogaerts and E. C. Neyts, "Plasma technology: an emerging technology for energy storage," ACS Energy Letters, vol. 3, pp. 1013-1027, 2018.
- W. Zhang, C. H. Chia, C. Cui, A. A. Umar, M. A. Mohamed, and M. R. Buyong, "A New Approach of Copper Oxide Electrode Fabrication for High Storage Pseudo-Type Supercapacitors," Available at SSRN 4830437.

# Use of ceramic oxides to reduce erosion of wind turbines due to solid particle impact.

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#### Abstract:

Over time, the use of composite materials has increased in industry and aerospace. They have mechanical properties very similar to those of steel, but with the advantage of being lighter and lower in cost. However, these materials pose a significant problem: when exposed to adverse weather conditions, they erode and their mechanical properties decrease. The use of ceramic oxides for mitigation has been very useful since they are highly versatile. They are non-conductive, non- oxidize upon contact with the environment, and non-photooxidize. This presents the use of aluminum oxide or alumina as an option. Samples are made with different weight-to-mass percentages ranging from 0.2, 0.4, 0.6, 0.8, and 1% with dimensions of 50 x 50 x 1 millimeters. 120-micron mesh silicon carbide is used as an erosion agent at time intervals of 30, 60, 120, 180, 240, and 360 seconds. The sample is placed perpendicular to the solid particle flow. Where scanning electron microscopy was used, in order to observe that by using a percentage of 0.8 and 1% of the mass of the test pieces, a reduction in the loss of mass and surface damage of the test piece was observed, causing the mechanical properties to be maintained for longer (Image 1).

**Keywords**: SEM, Erosion, Alumina, silicon carbide, Solid Particles.



**Figure 1**: The image shows how the increase in ceramic oxide reduces the loss of material in the test piece, allowing it to maintain its mechanical properties for longer, thus avoiding malfunction of the rotating element and, where appropriate, reducing the efficiency of a wind turbine.

- N. H. Arani, M. Eghbal, and M. Papini, "Numerical simulation of solid particle erosion of epoxy by overlapping angular particle impacts," Tribology Letters, vol. 68, no. 2, Apr. 2020, doi: 10.1007/s11249-020-01305-w.
- C. Samuel, M. Arivarasu, and P. Ram, "HighTemperature solid particle erosion behavior of laser powder bed fused Inconel 718," Journal of Tribology, vol. 144, no. 9, Mar. 2022, doi: 10.1115/1.4054052.
- M. Al-Bukhaiti, A. Abouel-Kasem, K. M. Emara, and S. M. Ahmed, "Particle shape and size effects on slurry erosion of AISI 5117 steels," Journal of Tribology, vol. 138, no. 2, Jan. 2016, doi: 10.1115/1.4031987.
- A. Abouel-Kasem, "Particle Size Effects on Slurry Erosion of 5117 steels," Journal of Tribology, vol. 133, no. 1, Dec. 2010, doi: 10.1115/1.4002605.

# Development of nanobiocatalytic systems toward the valorization of agri-food wastes

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## Abstract:

Agricultural residues, such as lignocellulosic biomass, and food wastes, have become a growing environmental concern due to their significant impact on ecosystems and human health [1]. Improperly managing these residues, such as open burning, contributes to air pollution, climate change, and soil degradation. The food industry, such as dairy, wine, and meat industry, is among the largest contributors to waste globally. Agricultural and food wastes and byproducts, often regarded as having minimal value, hold considerable potential for the of synthesis valuable compounds [2]. Valorization of these materials not only offers the ability to recover valuable bioactive compounds but also mitigates the environmental impact. Biocatalysis has emerged as a promising tool for managing agri-food by-products by enhancing the efficiency of biotransformation processes. Moreover, using immobilized biocatalysts on nanostructured supports offers the advantages of high biocatalyst maintenance (increased activity and stability in harsh conditions) and easy recovery and reuse of the biocatalysts, factors that improve the biotransformation processes, the cost-effectiveness of the procedures, and the promotion of circular economy [3].

Toward this aim, we report the development of nanobiocatalytic systems based on the immobilization of hydrolytic (e.g., cellulase, glucosidase, galactosidase) and oxidative (e.g., laccase, peroxidase) enzymes on green-produced nanomaterials. The synthesized nanobiocatalysts were evaluated for their catalytic activity, thermal stability, and reusability. Finally, the resulted nanobiocatlytic systems were applied for the biotransformation of agricultural by-products towards high-added value products with increased scientific and industrial interest.

**Keywords**: agricultural residues, food waste, enzymes, nanobiocatalysis, nanoparticles, biotransformation, bioactive compounds, valorization.



**Figure 1**: Figure illustrating the philosophy of a circular economy applied in the valorization of agri-food wastes using nanobiocatalystic systems for the production of high-added value products with potential exploitation.

#### **References:**

- Blasi, A., Verardi, A., Lopresto, C. G., Siciliano, S., & Sangiorgio, P. (2023), Lignocellulosic Agricultural Waste Valorization to Obtain Valuable Products: An Overview. *Recycling*, 8(4), 1–46.
- Ahmad, T., Esposito, F., Cirillo T. (2024), Valorization of agro-food by-products: Advancing sustainability and sustainable development goals 2030 though functional compounds recovery, *Food Biosci.*, 62, 105194-105206.
- Gkantzou, E., Chatzikonstantinou, A.V., Fotiadou, R., Giannakopoulou, A., Stamatis, H. (2021), Trends in the development of innovative nanobiocatalysts and their application in biocatalytic transformations, *Biotech. Adv.*, 51, 107738.

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# Development of Chymosin-Based Nanobiocatalyst through Immobilization on High Quality Few-Layer Bio-Graphene

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#### Abstract:

In this work, we report the green production of few-layer bio-Graphene (bG) through liquid exfoliation of graphite in the presence of bovine serum albumin. A range of experimental characterization techniques, including X-ray diffraction (XRD), atomic force microscopy (AFM), Ultraviolet-Visible (UV-Vis) and (FTIR) Fourier-Transform Infrared spectroscopies, were employed to evaluate the properties and the quality of the produced bio-Graphene. Microscopic characterization evaluated the quality of the produced nanomaterial, showing the presence of 3–4-layer graphene (Figure 1). Moreover, spectroscopic techniques also confirmed the quality of the resulted bG, as well as the presence of bovine serum albumin on the graphene sheets. bG was used to support the covalent and non-covalent immobilization of proteolytic enzyme chymosin (rennin). Several parameters potentially affecting the immobilization yield and enzyme-specific activity were tested, namely the support-toenzyme mass ratio, immobilization incubation time and incubation temperature. Immobilized chymosin showed higher activity the hydrolysis of milk k-casein than native chymosin at high temperature The storage, thermal and operational stability of the nanobiocatalyst was up to 2-fold higher compared to the non-immobilized biocatalyst.

Keywords: bio-graphene, rennin, green synthesis, nanobiocatalytic system, immobilization, enzyme.



few-layer

production

through liquid exfoliation of graphite in the presence of bovine serum albumin (BSA)

#### **References:**

 Alatzoglou, C., Patila, N., Giannakopoulou, A., Spyrou, K., Yan, F., Li, W., Chalmpes, N., Polydera, A.C., Rudolf, P., Gournis, D., Stamatis, H., (2023) Development of a Multi-Enzymatic Biocatalytic System through Immobilization on High Quality Few-Layer bio-Graphene *Nanomaterials* 13 (1), 127.

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bio-Graphene

(bG)



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