NANOTECH FRANCE 2021

NanoMetrology
2021

NanoMatEn
2021

Biotech
FRANCE
2021

NANOTECH / BIOTECH FRANCE 2021 AND JOINT VIRTUAL CONFERENCES

23 - 25 JUNE, 2021

BOOK OF ABSTRACTS

Organizer

Science Engineering Technology

SETCOR
Conferences & Exhibitions

Nanotech / Biotech / NanoMatEn / NanoMetrology 2021
Joint Virtual Conferences Program

23 - 25 June 2021 (GMT + 2 Time Zone)

June 23, 2021
Nanotech France session I.A

Virtual Conference Room 1

Session's Chairs:
Prof. Jacques Jupille, Institut des Nanosciences de Paris, France

10:00 -10:30	Exploiting Functional Materials for a Better Life **R.F.P. Martins**, S. Nandy and E.Fortunato	**Prof. Rodrigo Ferrão de Paiva Martins,** Nova Univ. of Lisbon, **Portugal**
10:30 -11:00	A sustainable alternative to flexible electronics based on metal oxide materials **E. Fortunato**, P. Barquinha, E. Carlos, R. Branquinho and R. Martins	**Prof. Elvira Fortunato**, New Univ. of Lisbon, **Portugal**
11:00 - 11:30	Synthesis of mesoporous organosilica nanoparticles for biomedical application **X. Cattoen**	**Dr. Xavier Cattoen**, CNRS-Néel Institute, **France**
11:30- 12:00	Structural and chemical analyses at the atomic scale of low dimensional materials by TEM **R. Arenal**	**Prof. Raul Arenal**, University of Zaragoza, **Spain**
12:00- 12:30	Trends in nanometrology using smart sensing with electron microscopes **L. C Gontard** and JJ Sáenz Noval	**Dr. Lionel Cervera Gontard,** Univ. of Cadiz, **Spain**
12:30-13:00	Identification and quantification of TiO2 anatase and rutile nanoparticles in binary mixture by Raman spectroscopy **A.M. Rossi**	**Dr. Andrea Mario Rossi**, National Institute of Metrological Research Turin, **Italy**
13:00 - 14:00	**Mid-Day Break / Posters Session**	

Nanotech - Session I.B:
Nanomaterials Fabrication / Synthesis / Charecterisation

Virtual Conference Room 1

Session's Chairs:
Prof. Jacques Jupille, Institut des Nanosciences de Paris, France
Dr. Anna Laura Pisello, University of Perugia, Italy
Prof. Raul Arenal, University of Zaragoza, Spain

14:00 - 14:30	Surface engineering of nanomaterials for water treatment **A.L.Daniel da Silva**	**Dr. Ana Luísa Daniel da Silva**, University of Aveiro, **Portugal**
14:30 - 14:45	Challenges on 2D materials in PVDF porous membranes designed to water desalination **A. Gugliuzza**, M. Frappa, F. Macedonio, G. Di Luca and E. Drioli	**Dr. Annarosa Gugliuzza**, Institute on Membrane Technology- CNR-ITM, **Italy**
14:45 - 15:00	Scalable and sustainable synthesis to produce iron oxide nanoparticles **L. Macera**, V. Daniele and G. Taglieri	**Dr. Ludovico Macera**, University of L'Aquila, **Italy**
15:00 - 15:15	Sustainable and eco-compatible nanolime based treatments in aqueous medium for the conservation of cultural heritage **V. Daniele**, L. Macera and G. Taglieri	**Dr. Valeria Daniele**, University of L'Aquila, **Italy**
15:15 - 15:30	Design, synthesis and characterization of polystyrene nanoparticles doped with lanthanide complexes for photoacoustic and near-infrared luminescence imaging **A. Kovalenko**, G. Collet, S. Natkunarajah, S. Lerondel, S. V. Eliseeva and S. Petoud	**Mr. Anton Kovalenko**, CNRS/UPR4301-Orléans, **France**
15:30 - 15:45	Tunable red-to-white luminescence of strontium vanadate **P. Wozny**, M. Runowski and S. Lis	**Mr. Przemysław Wozny**, Adam Mickiewicz University Poznan, **Poland**

15:45 – 16:00	Study of Cu coordination core in copper complexes grafted onto Au nanorods **I. Schiesaro**, I. Venditti, C. Battocchio, M. Pellei, C. Santini and C. Meneghini	**Ms. Irene Schiesaro**, Roma Tre University, **Italy**
16:00 - 16:30	**Afternoon Break / Posters Session**	
16:30 - 16:45	Detection of organophosphorous compounds with nanostructured microcantilever-based sensors **J-P. Brach**, G. Thomas, V. Keller and M. Comet	**Mr. Jean-Philippe Brach**, French-German Research Institute of Saint-Louis, **France**
16:45 - 17:00	Highly reproducible gram-scale CdSe/CdS giant-shelled nanocrystal synthesis with tunable particle geometry **S. Krohn**, A. Mews and J. S. Niehaus	**Ms. Sonja Krohn**, Fraunhofer IAP-CAN, **Germany**
17:00 - 17:15	Nanofibrillar Green Composites of Polylactide/Polyamide Produced in Situ Due to Shear Induced Crystallization R. Hosseinnezhad, **I. Vozniak**, J. Morawiec and A. Galeski	**Dr. Iurii Vozniak**, Polish Academy of Sciences-Lodz, **Poland**
17:15 - 17:30	Multi-functional Natural Fiber Composites for Shear Loading **S. Yang**, V.B. Chalivendra and Y. Kim	**Prof. Yong K. Kim**, Univ. of Massachusetts Dartmouth, **USA**
17:30 - 17:45	The effect of sintering temperature on the electro physical properties of Silicon-polymer based composite Varistors M. Dadgar and **F. Tayefi Ardebili**	**Ms. Faranak Tayefi Ardebili**, Jagiellonian University, **Poland**
17:45 - 18:00	The effect of sintering pressure on the electro physical properties of Silicon-polyaniline–polyethylene composite Varistors F. Tayefi Ardebili and **M. Dadgar**	**Mr. Meysam Dadgar**, Jagiellonian University, **Poland**
18:00 - 18:15	MBE Growth and NC-AFM/KPFM characterization of 2 D materials under UHV environnement : graphene and silicene. **H. Ichou** and D.Martrou	**Mr. Hamza Ichou**, Paul Sabatier University, **France**
18:15 – 18:30	Optimization of the terminations and stability of polyynes through ns-pulsed laser ablation in organic solvents **P. Marabotti**, S. Peggiani, R. A. Lotti, A. Facibeni, P. Serafini, V. Russo, A. Li Bassi and C. S. Casari	**Mr Pietro Marabotti**, Polytechnic University of Milan, **Italy**
18:30 – 18:45	Electorospun nanofibers with photocatalytic particles for carbon sorption **Y. Tskhe**, M. Buzgo and A. Simaite	**Ms. Yekaterina Tskhe**, University of Montpellier, **France**
18:45 – 19:00	Silica and alumina-silica based aerogels reinforced with aramid fibres as promising candidates for Space applications **M.E. Ghica**, C.M.R. Almeida, L. Rebelo, G. Cathoud-Pinheiro and L. Durães	**Dr. Mariana E. Ghica**, University of Coimbra, **Portugal**

June 23, 2021
Biotech France session I.C

Virtual Conference Room 2

Session's Chairs:
Prof Ralf Takors, University of Stuttgart, Germany
Dr. Alfred Fernández-Castané, Aston University, UK
Dr. Ioscani Jiménez del Val, University College Dublin, Ireland

14:00 - 14:30	Synthetic Biology for a Sustainable World **R.I Kitney**	**Prof. Richard Ian Kitney**, Imperial College London, **UK**
14:30 - 15:00	Microbial Electrochemical Technologies Enable New Biotechnologi-cal Processes **J.O Krömer**	**Dr. Jens O. Krömer,** Helmholtz Centre for Environmental Research - UFZ, **Germany**
15:00 - 15:30	The potential of microbial biotechnology toward a low-carbon bioeconomy **A. Fernández-Castané** and P. Thornley	**Dr. Alfred Fernández-Castané**, Aston University, **UK**
15:30 - 16:00	Scaling up from lab to industrial scale minimizing performance loss: From simulation to strain engineering of E. coli M. Ziegler, J. Zieringer, M. Wild and **R. Takors**	**Prof Ralf Takors,** University of Stuttgart, **Germany**
16:00 - 16:30	**Afternoon Break / Posters Session**	
16:30 - 17:00	Model-informed biopharmaceutical glycoengineering **I.Jiménez del Val**	**Dr. Ioscani Jiménez del Val,** University College Dublin, **Ireland**
17:00 - 17:30	The potential of hybrid process modeling and digital twins to master the goals of industry 4.0 in bioprocessing **M. Sokolov**; H. Narayanan; M. von Stosch; Morbidelli and M.Butte	**Dr. Michael Sokolov**, DataHow AG, **Switzerland**
17:30 - 17:45	Gasification of biomass: Characterisation of spelt husk briquette and pellet. **A. Halidu**, E. Neofytou, P. Bilsborrow and P. Phan Anh	**Mr. Abubakar Halidu**, Newcastle University, Newcastle upon Tyne, **UK**
17:45 – 18:00	Removal of Poisonous Arsenic (As) from Drinking Water in Developing Countries by using Wasted Coffee Beans **M.Minagawa**, H.Akashi, Y.Osamura and D.Adolphe	**Mr. Gakusai Minagawa**, NPO- Dream-Create-Laboratories, **Japan**

June 24, 2021
Nanotech / NanoMetrolgy joint session II.A:
Workshop on VIMMP project - Virtual Materials Marketplace (H2020 GA 760907)

Virtual Conference Room 1

Session's Chairs:
Dr. Welchy Leite Cavalcanti, IFAM, Germany
Dr. Michael Hoffmann, IFAM, Germany

08:30 - 09:00	Knowledge representation for materials modelling marketplaces **M. T. Horsch**, S. Chiacchiera, M. A. Seaton, I. T. Todorov, P. Klein, N. A. Konchakova, C. Niethammer, J. Vrabec, G. Mogni, D.Toti, G. Goldbeck, P. Schiffels and W. L. Cavalcant	**Dr. Martin Thomas Horsch,** High Performance Computing Center Stuttgart, **Germany**
09:00 - 09:30	New concepts of assembling fibrous biopolymer scaffolds to control cell interactions **D. Brüggemann**	**Prof. Dorothea Brüggemann**, University of Bremen, **Germany**
09:30 - 09:45	Numerical simulation of food emulsion production: the mayonnaise case **A. Buffo**, M. Ferrari, G. Boccardo, M. Vanni and D. Marchisio	**Prof. Antonio Buffo**, The Polytechnic University of Turin, **Italy**
09:45 - 10:00	Dispersive mixing of filler agglomerates in a polymer compounding operation: A CFD-DEM investigation **G. Frungieri**, G. Boccardo, A. Buffo, D. Marchisio, A. Karimi-Varzaneh and M. Vanni	**Dr. Graziano Frungieri**, Polytechnic University of Turin, **Italy**
10:00 - 10:15	Salt-induced self-assembly of fibrinogen nanofibers: How the development of new bio-materials can benefit from a virtual materials marketplace **S. Stamboroski**, W. L. Cavalcanti and D. Brüggemann	**Dr. Stephani Stamboroski**, Fraunhofer Institute for Manufacturing Technology and Ad. Materials, **Germany**
10:15 -10:30	Mesoscopic Modelling of Interactions of Structured Fluids with Soft Surfaces **K. Sindelka** and M. Lísal	**Dr. Karel Sindelka**, Institute of Chemical Process Fundamentals- Czech Academy of Sciences, **Czech Republic**
10:30 -10:45	Calculation of the work of adhesion of polyisoprene on graphite by molecular dynamics simulations **M. Chiricotto**, G. Giunta, H. A. Karimi-Varzaneh and P. Carbone	**Dr. Mara Chiricotto**, The University of Manchester, United Kingdom
10:45 - 11:00	**Morning Break / Posters Session**	

Nanotech France- Focused session on Nanocoatings/ Thin films and nanostructured surfaces

Chairs:
Prof. Jacques Jupille, Institut des Nanosciences de Paris, France
Prof. Maria Gioti, Aristotle University of Thessaloniki, Greece

11:00 - 11:15	Synthesis of Nanostructured Metallic Foams by Plasma Electrolysis Deposition **J. Pinot**, R.Botrel, F.Durut, L.Reverdy, L.Pescayre and V.Vignal	**Mr. Julien Pinot**, CEA, **France**
11:15 - 11:30	One-step Templateless Electrosynthesis of Nanostructured PEDOT films **D. Wang** and C. Debiemme-Chouvy	**Ms. Dantong Wang**, CNRS-Sorbonne University, **France**
11:30 - 11:45	Influence of element composition on thermal stability and oxidation resistance of Ti-Cr-Mo-Ni-N coatings **A. Chernogor**, I. Blinkov and A. Volkhonskiy	**Mr. Alexey Chernogor**, NUST "MISiS", **Russia**
11:45 - 12:00	Synthesis of Can+1MnnO3n+1 thin films by Pulsed-Laser Deposition **B. M. Silva**, J. Oliveira, T. Rebelo, L. Francis, J. H. Belo, A. Lopes, J.P. Araújo, L. D. Francis and B. G. Almeida	**Ms. Bruna Silva**, Univ. Minho, **Portugal**
12:00 - 12:15	Using 1D nanoimprint master templates to fabricate variable 2D nanogratings in indium tin oxide **J. Buhl**, D. Yoo and M. Gerken	**Dr. Janek Buhl**, Kiel University, **Germany**

12:15 - 12:30	Thermal Laser Epitaxy – Ultrapure Epitaxy beyond PLD and MBE **W. Braun**, D. Yeong Kim, T.J. Smart, H. Boschker, S. Smink, L.N. Majer and J. Mannhart	**Dr. Wolfgang Braun**, Max Planck Institute for Solid State Research, **Germany**
12:30 - 12:45	Spectroscopic ellipsometry studies on solution processed OLED devices: optical properties and interfacial layers **M. Gioti**	**Prof. Maria Gioti**, Aristotle University of Thessaloniki, **Greece**
12:45 - 13:00	Preparation of High Density Polyurethane Surfaces for Metalliza-tion **B. Aykac**, Y. Oz, I. Karakaya and M. Erdogan	**Mrs. Büşra Aykaç**, Turkish Aerospace., Advanced Materials Process and Energy Technologies Center, **Turkey**
12:30 - 14:00	**Mid-Day Break / Posters Session**	

June 24, 2021

Nanotech/ Nanometrology - Session II.B:
Nanomaterials Modelling and Characterisation

Virtual Conference Room 1

Session's Chairs:
Prof. Eden Mamut, Ovidius University of Constanta, Romania
Prof. Antonio Buffo, The Polytechnic University of Turin, Italy

14:00 - 14:30	How can we "see" and "feel" the dynamics at nanoscale: A scanning probe microscope approach **Q. Zou**	**Prof. Qingze Zou**, Rutgers University, USA
14:30 - 15:00	Manufacture and calibration of high stiffness AFM cantilevers **J. Bowen**, D. Cheneler and J. Vicary	**Dr. James Bowen** Univ. of Birmingham, **UK**
15:00 - 15:15	Nanoscale monitoring of the molecular complexes structural and me-chanical changes by use of the AFM **J. Pribyl**, J. Vítecek and L. Kubala	**Dr. Jan Pribyl**, CEITEC MU, Masaryk University, **Czech Republic**
15:15 - 15:30	SiC Nanowire Foams for pressure detection **Y. Chen**, Y. Xia and Y. Zhu	**Mr. Yu Chen**, University of Exeter, **UK**
15:30 - 15:45	In situ generation of sub-10 nm silver nanowires under electron beam irradiation in a TEM **L. D. Francis** and J. Li	**Dr. Leonard D. Francis**, International Iberian Nanotechnology Laboratory **Portugal**
15:45 - 16:00	Challenges on inline monitoring of nanosized polymer materials **S. Schlappa**, L. Bressel, M. Münzberg and A. Bergner	**Ms. Stephanie Schlappa**, University of Potsdam, **Germany**
16:00 - 16:30	**Afternoon Break / Posters Session**	
Session's Chairs: **Dr. James Bowen Univ. of Birmingham, UK**		
16:30 - 16:45	Comb-referenced interferometry in nanopositioning and nano-measuring machines **U. Blumroder**, P. Kochert, T. Fröhlich, R. Füßl, I. Ortlepp, U. Gerhardt, R. Mastylo, J. Flügge, H. Bosse and E. Manske	**Dr. Ulrike Blumroder**, Ilmenau University of Technology, **Germany**
16:45 - 17:00	Nanoplastics characterization at the biological interface **S. Ducoli**, S. Federici, L. Paolini, A. Radeghieri, P. Bergese, E. Bontempi and L.E. Depero	**Ms. Serena Ducoli**, University of Brescia, **Italy**
17:00 - 17:15	Disease Control via Mosquito Nano-Tech-Repellents **J. Bozeman**	**Dr. James Bozeman**, American University of Malta, **Malta**
17:15 - 17:30	Molecular Dynamics of ion transport through SWCNTs: a focus on water model and pore geometrical parameter effects. **A. Mejri**, G. Herlem and F. Picaud	**Dr. Alia Mejri**, Bourgogne-Franche-Comte University, **France**.
17:30 - 17:45	Ring-o-rings: joining the ends of poly[M]-catenanes to control supramolecular torsion **L. Tubiana**, F. Ferrari and E. Orlandini	**Dr. Luca Tubiana**, University of Trento, **Italy**
17:45 - 18:00	Experimental study of colloidal particles confined in a droplet formed in a microfluidic channel **L. Chagot**, M. Kalli and P. Angeli	**Dr. Loïc Chagot,** University College London, **UK**
18:00 - 18:15	The Effect of Particle Loading, Surfactant Concentration and Soni-cation Time on The Wettability Of Multi-Walled Carbon Nanotubes Based Nanofluid **M.A. Hassan**, T .A. Osman, F. Elharouni, H.A. Kishawy, H. Hegab and A.M.K. Esawi	**Mr. Mohamed A. Hassan**, The American University in Cairo, **Egypt**.
18:15 - 18:30	Colloidal Suspension of Silver Nanoparticles for Random Dispersion of LASER Beams **E. Mamut**, L. Oancea, G. Prodan and A. Enache	**Prof. Eden Mamut**, Ovidius University of Constanta, **Romania**

June 24, 2021 Nanotech / Biotech Joint session II.C		
Virtual Conference Room 2		
Session's Chairs: Dr. Claire Wilhelm, Paris Diderot University, France		
09:30 - 10:00	Self-assembling supramolecular dendrimer nanosystems for biomedical applications **L. Peng**	**Dr. Ling Peng**, CNRS, Aix-Marseille University, **France**
10:00 - 10:30	The interplay of efficiency and biodegradation for inorganic nanohybrids in cancer or regenerative therapies. **C.Wilhelm**	**Dr. Claire Wilhelm**, Paris Diderot University, **France**
10:30 - 11:00	**Morning Break / Posters Session**	
11:00 - 11:15	Fundamental Chronobiological Changes in Nanostructure of Bone Tissue **A. A. Pavlychev**, X.O. Brykalova and N.N. Kornillov	**Prof. Andrey Pavlychev**, St.Petersburg State University, **Russia**
11:15 - 11:30	Antibacterial nanostructured coatings on high-touch surfaces to prevent pathogen transmission in hospital settings. **M. Stanzione**, G. G. Buonocore, M. Lavorgna, A.M. Marcelloni, I. Amori, A.R. Proietto, A. Chiominto, E. Paba and A. Mansi	**Dr. Mariamelia Stanzione**, CNR - National Research Council, **Italy**
11:30 - 11:45	Flexible NO2-Functionalized N-Heterocyclic Carbene Monolayers on Au (111) Surface **S. Dery**, S. Kim, F.D. Toste and E. Gross	**Mr. Shahar Dery**, Hebrew University, **Israel**
11:45 - 12:00	Interaction of bacteriophage lambda with lipid Langmuir Monolayers **A. Leader**, M. Reches and D. Mandler	**Mrs. Avia Leader**, Hebrew University, **Israel**
12:00 - 12:15	Integrated approach for exposure and health effects monitoring of engineered nanomaterials in workplaces and urban areas **A. Progiou** , E. Bergamaschi, I. Guseva-Canu, C. Fito, M. Domat, S. Lopez and J. Friesl	**Dr. Athena Progiou**, AXON Enviro-Group, **Greece**
12:15 - 14:00	**Mid-Day Break / Posters Session**	

June 24, 2021
Nanotech / Biotech - Session II.D:
Nanotechnology for life science- Biosensors, Diagnostics and Imaging

Virtual Conference Room 2

Session's Chairs:
Dr. Ling Peng, CNRS, Aix-Marseille University, France
Prof. Qingze Zou, Rutgers University, USA

14:00 - 14:30	Molecular Imaging with Nanodiagnostics **F. Kiessling**	**Prof. Fabian Kiessling,** RWTH Aachen University, **German**
14:30 - 15:00	Nanosensorics for clinical applications **L. Baraban**	**Dr. Larysa Baraban**,, Helmholtz Center Dresden Rossendorf, **Germany**
15:00 - 15:30	Magnetic Nanoparticles in Biomedical Applications **T. Sen**	**Dr. Tapas Sen**, University of Central Lancashire, **UK**
15:30 - 15:45	Functionalized porous materials for the detection of low concen-trated metabolites and drugs D. Bergé-Lefranc, C. Belliardo, T. N. T Phan, D. Rayeroux, C. Pardanaud, A. Merlen, K. Mabrouk, M. Rollet, D. Gigmes, R. Denoyel and **V. Hornebecq**	**Dr. Virginie Hornebecq**, Aix-Marseille University, **France**
15:45 - 16:00	Towards a new generation of electrical biosensors based on 2D silicon nanowire networks for DNA and Thrombin detection M. Vallejo Perez, C. Ternon, F. Morisot, C. Gondran, K. Gorgy, N. Spinelli, B. Salem, M. Mouis, X. Mescot, L. Rapenne and **V. Stambouli**	**Mrs. Valerie Stambouli**, CNRS- LMGP Grenoble INP, **France**
16:00 - 16:30	**Afternoon Break / Posters Session**	
16:30 - 16:45	Engineered Graphene decorated Aluminum-based plasmonic nanostructures for biosensing applications in the optical Communication band S. Shukla, J. Yadav1, S. Jain and **P. Arora**	**Mr. Pankaj Arora**, Birla Institute of Technology and Science, **India**
16:45 - 17:00	Electro-Spun Silk-CNT Fibers to Stimulate Fibroblasts for Connective Tissue Repair **R. Wang**, N. Chi, S. Zheng, E. Clutter and C.Rathnayake	**Prof. Rong Wang**, Illinois Institute of Technology, **USA**
17:00 - 17:15	Engineering Gold Nanoshells for Targeted Therapeutics & Point-of-Care Diagnostic Technologies **A. E. Saunders** and S. J. Oldenburg	**Dr. Aaron E. Saunders**, nanoComposix, **USA**

June 25, 2021 **NanoMatEn - Session III.A:** **Nanomaterials for Energy / Nanoelectronics**		
Virtual Conference Room 1		
Session's Chairs: **Dr. Xavier Cattoen, CNRS-Néel Institute, France** **Prof. Rodrigo Ferrão de Paiva Martins, Nova Univ. of Lisbon, Portugal**		
09:00 - 09:30	Nanowire solar cells: Challenging fundamental limits **J. Haverkort**	**Prof. Jos Haverkort**, Eindhoven University of Technology, **Netherlands**
09:30 - 10:00	Nanothermometry Through Light Emission **L.D. Carlos**	**Prof. Luís Dias Carlos**, University of Aveiro, **Portugal**
10:00 - 10:30	Human-centered multiphysics approach for improving livability in urban areas: the role of smart materials and novel metrics for cities resilience to anthropogenic environmental forcing **A.L. Pisello**	**Dr. Anna Laura Pisello**, University of Perugia, **Italy**
10:30 - 11:00	**Morning Break / Posters Session**	
Session's Chairs: **Prof. Luís Dias Carlos, University of Aveiro, Portugal** **Prof. Maria Gioti, Aristotle University of Thessaloniki, Greece**		
11:00 - 11:15	Efficient oxygen evolution and gas bubble release achieved by a low-gas bubble-adhesion iron-nickel vanadate electrocatalyst **K. Dastafkan** and C. Zhao	**Mr. Kamran Dastafkan**, The University of New South Walses, **Australia**
11:15 - 11:30	Entrapped carbon quantum dots in a composite for oxygen reduction in anion exchange membrane fuel cells **A. R. Nallayagari**, E. Sgreccia, P. Knauth and M. L. Di Vona	**Ms. Ashwini R. Nallayagari**, University of Rome Tor Vergata, **Italy**
11:30 - 11:45	Engineering of Electrode Materials and Interfaces in Perovskite Photovoltaics **L. Kavan**	**Prof. Ladislav Kavan,** J. Heyrovsky Institute of Physical Chemistry, **Czech Republic**
11:45 - 12:00	CuCrO2 thin films out of stoichiometry as semi-transparent Hole Transparent Layer in performant and recyclable hybrid solar cells **L. Bottiglieri**, A. Nourdine, J. Resende, C. Jimenez and J.L. Deschanvres	**Mr. Lorenzo Bottiglieri,** LMGP/CNRS, Univ. Grenoble Alpes, **France**
12:00 - 12:15	Fluorescent and water-dispersible ternary alloyed Cu- and Al-co-doped ZnSeS/ZnS QDs **S. Mabrouk**, H. Rinnert, L. Balan, G. Medjahdi, R. Ben Chaabane and R. Schneider	**Mrs. Salima Mabrouk**, University of Lorraine, **France**
12:15 - 12:30	High performance 2D micro-supercapacitor electrode composed of graphene with polydopamine as inserts **A. Bouzina**, H. Perrot, O. Sel and C Debiemme-Chouvy	**Mr. Adnane Bouzina**, CNRS- Sorbonne University, **France**
12:30 - 12:45	PEO-based porous silica hybrid materials as solid electrolytes for all-solid-state lithium ion batteries C. Lebouin, **K. Maouacine**, L. Pasquini, T. N. T Phan and V. Hornebecq	**Mr. Koceila Maouacine**, Aix-Marseille University, **France**
12:45 - 13:00	CNT and Graphene based Nanocomposite for Enhancing the Heat Transfer Processes in Hybrid Solar Panels **E. Mamut**, L. Oancea 1, O.F. Ghinea	**Prof. Eden Mamut**, Ovidius University of Constanta, **Romania**
13:00 - 14:00	**Mid-Day Break / Posters Session**	
Session's Chairs: **Prof. Eden Mamut, Ovidius University of Constanta, Romania** **Prof. Rodrigo Ferrão de Paiva Martins, Nova Univ. of Lisbon, Portugal**		
14:00 - 14:15	1D and 2D confinement in CsPbBr3 perovskite nanocrystals V. Steinmetz, J. Ramade, L. Legrand, T. Barisien, F. Bernardot, E. Lhuillier, I. Saïdi, A. Ghribi, K. Boudjaria, C. Testelin and **M. Chamarro**.	**Dr. Maria Chamarro**, Sorbonne University, **France**

14:15 - 14:30	Fabrication of Polarized Emissive Optical Devices Based on Anisotropic Nanomaterials **C. Castillo Delgadillo**, H. Schlicke, J. Niehaus, H. Weller and A. Mews	**Mr. Christian Castillo Delgadillo**, Fraunhofer Center for Applied Nanotechnology, **Germany**
14:30 - 14:45	Gas sensors based on PbS colloidal quantum dots **F. Mitri**, A. De Iacovo, L. Colace, M. De Luca and A. Pecora	**Mrs. Federica Mitri**, University Roma Tre, **Italy**
14:45 - 15:00	Wavelength Selective Photodetectors based on PbS Colloidal Quantum Dots as Photoactive Layers and Optical Filters **C. Venettacci**, A. De Iacovo, L. Colace and C. Giansante	**Dr. Carlo Venettacci**, University Roma Tre, **Italy**
15:00 - 15:15	OLEDs on Flexible Substrates Nanostructured with UV-Nanoimprint Lithography **Y. Murat**, K. Petersons, J. Buhl, L. Lindvold, L. Yde, J. Stensborg and M. Gerken	**Dr. Yolande Murat**, Kiel University, **Germany**
NanoMatEn - Session III.B **Nanotechnology for Environmental Application / Water treatment**		
Session's Chairs: **Dr. Chedly Tizaoui, Swansea University, UK** **Dr. Herman Mansur, Federal University of Minas Gerais (UFMG), Brazil** **Dr. Ana Luísa Daniel da Silva, University of Aveiro, Portugal**		
15:15-15:45	Nanotechnology for Water Treatment **C. Tizaoui** and S. Farooq	**Dr. Chedly Tizaoui**, Swansea University, **UK**
15:45-16:00	Nanocomposite Gels for Plugging of Fractures in Carbonate Oil Reservoirs **I. Fjelde** and A.A. Ogienagbon	**Prof. Ingebret Fjelde**, NORCE Norwegian Research Centre, **Norway**
16:00 - 16:30	**Afternoon Break / Posters Session**	
16:30 - 16:45	Electroless Metallisation of Textiles using Copper-based Nanopar-ticle Catalysts for Inkjet Printing **D. Fox**, G.T.Pourian Azar, L. Krishnan and A.J. Cobley	**Dr. Daryl Fox**, Coventry University, **USA**
16:45 - 17:00	Application of multifunctional nanoparticles for cellulose fibers modifications. **M. Skwierczynska**, M. Runowski, P. Kulpinski and S. Lis	**Ms. Małgorzata Skwierczynska**, Adam Mickiewicz University Poznan, **Poland**
17:00 - 17:15	Quaternary Semiconductor Quantum Dots/Magnetic Iron Oxide Nanoparticles Covalently Coupled through Biopolymer Ligands as Multifunctional Nanohybrids: Insights of Photocatalytic Activity for Degradation of Water Pollutants A. G. Leonel, A. A. P. Mansur, J. C.Jr. Amaral and **H.S. Mansur**	**Dr. Herman Mansur**, Federal University of Minas Gerais (UFMG), **Brazil**
17:15 - 17:30	ZnO / FexOy for water depollution by photocatalysis under natural sunlight **M. Le Pivert**, N. Martin and Y. Leprince-Wang	**Mrs Marie Le Pivert**, Université Paris-Est-Marne-la-Vallée, **France**
17:30 - 17:45	Doped ZnAl-CO3 layered double hydroxides as DeNOx photocatalysts with enhanced visible light harvesting **A. Pastor**, F. Rodriguez-Rivas, G. de Miguel, M. Cruz-Yusta, F. Martin, I. Pavlovic and L. Sánchez	**Mr. Adrian Pastor**, Cordoba University, **Spain**
17:45 - 18:00	Transformation of CO2/bicarbonates into formate over a Ni@Ni(OH)2 nanocatalyst **K. Philippot**, L. Peres, X.-P. Fu , J. Esvan, C. Amiens and N. Yan	**Dr. Karine Philippot**, LCC-CNRS Toulouse, **France**

June 25, 2021

Nanotech / Biotech - Session III.C
Nanotechnology for drug and gene delivery

Virtual Conference Room 2

Session's Chairs:
Dr. Tapas Sen, University of Central Lancashire, UK
Prof Lucia Gutiérrez Marruedo, University of Zaragoza, Spain

09:15 - 09:30	Development of multifuntional MRI immunomodulating theranostic agents for Cancer **M. Khan**, S.Boumati, A.T. Diallo, N.Djaker, Bich-Thuy Doan and J.Spadavecchia	**Ms. Memona Khan**, University Paris 13**, France**
09:30 - 09:45	Hybrid carbon nanotubes/gold nanostars for photothermal cancer treatment **R. Soltani**, A. Abou-Hassan, C.Wilhelm, A. Bianco and C. Ménard-Moyon	**Ms. Rym Soltani**, University of Strasbourg, **France**
09:45 - 10:00	Design and Evaluation of Thermosensitive Liposomes Encapsulating Nedaplatin and Picoplatin with Controlled-Release and Enhanced Anticancer activity **S.A. Fahmy**, M. Alawak, E. Preis, A. Abu Dayyih, U. Bakowsky and T. Shoeib	**Dr. Sherif A. Fahmy**, American University in Cairo **Egypt**
10:00 - 10:15	Isolation of extracellular vesicles from Brassica oleracea L. (Broccoli) and study of their effect on the metabolic activity of tumor cell lines **M.N. Hossain**, V. De Leo, R. Tamborra, L. Catucci, M. Conese and S. Di Gioia	**Mr. Md Niamat Hossain**, University of Foggia, **Italy**
10:15 - 10:30	Evaluation of doxorubicin-loaded iron oxide nanoparticles synthesis and in vitro cytotoxicity on 4T1 tumorigenic epithelial cell lines **N. Maisuradze**, J. Markhulia, Sh. Kekutia, T. Tsertsvadze, V. Mikelashvili, L. Saneblidze, N. Leladze, M. Kriechbaum and L. Almasy	**Ms. Nino Maisuradze**, Ivane Javakhishvili Tbilisi State University, **Georgia**
10:30-11:00	**Morning Break / Posters Session**	
11:00 - 11:30	Magnetically-Driven Drug Release from Magnetosomes: Challenges and Applications A.C. Moreno-Maldonado, A. Toro-Córdova, M.R. Ibarra and **G.F. Goya**	**Dr. Gerardo F. Goya**, University of Zaragoza, **Spain**
11:30 - 11:45	Understanding of in vivo behavior of nanosystem based on magnetic nanoparticles **A.G. Pershina**, O.Y. Brikunova, L.V. Efimova, A.M. Demin, V.A. Naumenko4, E.S. Khmelevskaya, V.P. Krasnov and L.M. Ogorodova	**Dr. Alexandra G. Pershina**, Siberian State Medical University, **Russia**
11:45 - 12:00	Bioencapsulation capabilities of HepE Nanoparticles and their medical Applications **C-C. Chen**, M.A. Baikoghli, L-A. Chen, R. H. Cheng	**Dr. Chun-Chieh Chen**, University of California Davis, **USA**
12:00 - 12:15	Modified zinc oxide nanoparticles as potential drug carriers **J. Pulit-Prociak**, O. Długosz, A. Staroń and M. Banach	**Dr. Jolanta Pulit-Prociak**, Cracow University of Technology, **Poland**
12:00 - 14:00	**Mid-Day Break / Posters Session**	

June 25, 2021

Nanotech / Biotech - Session III.D:
Nanotechnology for life science

Virtual Conference Room 2

Session's Chairs:
Dr. Gerardo F. Goya, University of Zaragoza, Spain
Dr. Larysa Baraban, Helmholtz Center Dresden Rossendorf, Germany

14:00 - 14:30	Pancreatic cancer treatment using magnetic hyperthermia **L. Gutiérrez Marruedo**	**Prof Lucia Gutiérrez Marruedo**, University of Zaragoza, **Spain**

14:30 - 14:45	Nanoemulsions stabilized by protein to encapsulate curcumin for a topical application. **G. Mekhloufi**, N. Vilamosa and F. Agnely	**Dr. Ghozlene Mekhloufi**, University Paris Saclay, **France**
14:45 - 15:00	Elaboration of the size-controlled polymeric nanomaterials; Rifampicin encapsulation and in-vitro release studies **J. Abdurahim**, C.A. Serra and M. Vauthier	**Mr. Javid Abdurahim**, University of Strasbourg, **France**
15:00 - 15:15	Co-adsorption and co-release of 5-fluorouracil and naproxen using pH-sensitive mesoporous silica particles E. Beňová, D. Buric, **D. Bergé-Lefranc**, V. Zeleňák and V. Hornebecq	**Mr. David Berge-Lefranc**, Aix Marseille Univ, **France**
15:15 - 15:30	Towards Smart Drug Delivering Systems: On the Absorption of Lap-onite colloids onto lipid Cubosomes **F. Ferdeghini**, C. Rerzki-Vérité, F. Cousin and F. Muller	**Dr. Filippo Ferdeghini**, ECE Paris, **France**
15:30 - 15:45	Poloxamer prodrug-based delivery of a pharmacologically enhanced camptothecin agent as an experimental therapy for drug-resistant neuroblastoma I.S. Alferiev , D. Guerrero, F. Nguyen, P. Guan, V. Kolla, D. Soberman, I. Fishbein, G.M. Brodeur and **M. Chorny**	**Dr. Michael Chorny**, The Children's Hospital of Philadelphia, **USA**
15:45 - 16:00	Captopril-loaded polymeric nanoparticles for the treatment of pediatric diseases **N. Nieto González**, A. Obinu, E. Gavini, P. Giunchedi, G. Cerri, J. Molpeceres and G.Rassu	**Ms Noelia Nieto González**, University of Sassari, **Italy**
16:00 - 16:30	**Afternoon Break / Posters Session**	
16:30 – 16:45	Application of Rose Bengal in the absence of light: targeting and treating melanoma via dermal delivered Rose Bengal-transfersomes **S. Demartis**, A. Obinu, G. Rassu, S. Murgia, L. Casula, P. Giunchedi and E. Gavini	**Ms. Sara Demartis**, University of Sassari, **Italy**
16:45 – 17:00	Scrutinizing nanoparticle-membrane interactions: Effects of the biomolecular corona, particle size and flow **C. J. Richards**, W. H. Roos and C. Åberg	**Ms. Ceri Richards**, University of Groningen, **Netherlands**
17:00 – 17:15	Novel applications of nanobiotechnology to decipher cell-materials and cell-cell interactions **O. Valentina**, I.L. Moldero, A. Chandra, F. Gentile, L. Moroni, and L.L. del Mercato	**Dr. Valentina Onesto**, CNR-NANOTEC, **Italy**

Posters Virtual Session

Posters are being displayed through the Virtual event solution.
Discussions are to be done through the system chat features available to the attendees.

N.	Title	Author/Affiliation/Country
1.	Synthesis of Stretchable and Environmentally Stable Conjugated Polymer PEDOT using a Random Copolymer with Modified Acid Template **Y. Kim**, J. Kim, H. Lee, C. Park, S. Im and J.H. Kim	**Mr. Youngno Kim**, Yonsei University, **Rep. of Korea**
2.	Optical properties and enhancement of Raman scattering of gold nanostructured arrays elaborated by scanning probe lithography **P. Taugeron**, M. Rahmani, N. Delorme and J.-F. Bardeau	**Mr. Pierre Taugeron**, Le Mans University, **France**
3.	The effect of nanofiller on the production of high performance multilayer fine-fibrous filter material by application of fused deposition modeling V.Beloshenko, N.Rezanova, N.Sova, R.Iskandarov and **A.Vozniak**	**Dr. Alina Vozniak**, Polish Academy of Sciences- Lodz, **Poland**
4.	Morphology, Thermal and Mechanical Properties of Polylactide Blends with Glycidyl Methacrylate-grafted Polypropylene **J. Su Lee** and Y. G. Jeong	**Ms. Ji Su Lee**, Chungnam National University, **Rep. of Korea**
5.	Thermally Conductive Polyimide-based Composites Films with Low Dimensional Ceramic Nanofillers **G.H. Hwang** and Y.G.Jeong	**Dr. Gyu Hyun Hwang**, Chungnam National University, **Rep. of Korea**
6.	Aromatic Poly(ether amide)s-derived Carbon Nanofiber Webs for Self-standing and Binder-free Supercapacitor Electrode Materials **Y.S. Kwon** and Y.G.Jeong	**Mr. Young Seung Kwon**, Chungnam National University, **Rep. of Korea**
7.	Preparation and characterization of carbon containing composite films on Al-Zn-Mg alloy using steam coating **T. Ishizaki**, H.Muto and Y. Nagashima	**Prof. Takahiro Ishizaki**, Shibaura Institute of Technology, **Japan**
8.	Synthesis and Characterization of Cu2S – TiO2 Heterostructures with Enhanced Photophysical Properties. **S. Al Suhaibani**, M. Abdelnaby and M. Zeama	**Mr. Sulaiman Al Suhaibani**, King Fahad University of Petrelouem and Minerals, **Saudi Arabia**
9.	Impact of pH on adsorption of hydrogen on Pt in aqueous phase **X. Chen**, Y. Liu and J. A. Lercher	**Mr. Xi Chen**, Technical University of Munich, **Germany**
10.	Optically Mapping Temperature in the Vicinity of Gold Nanorods **T. Albogami**, K. Critchley, Z.Y Ong, and S.D Evans.	**Mrs.Tahani Albogami**, University of Leeds, **UK**.
11.	Structural analysis of AlInN layers deposited on Si(100) and Si(111) via reactive RF sputtering **M. Sun**, R. Blasco, S. Valdueza-Felip, F. B. Naranjo, M. de la Mata and S. I. Molina	**Mr. Michael Sun**, University of Alcala, **Spain**
12.	Recording Material Synthesis Images and Processing with a Script for Data Visualization **D. Sousa**, J. C. Lima and I. Ferreira	**Mr. David Sousa**, NOVA School of Science and Technology, **Portugal**
13.	3D-printed Bioactive Scaffolds for Bone Regeneration Bearing Carbon Dots for Bioimaging Purposes A. Saranti, A. Tiron-Stathopoulos, C. Gioti, A. Ioannou, A. Vassilakopoulou, M.A. Karakas-sides, I. Koutselas and **K. Dimos**	**Prof. Konstantinos Dimos**, University of Patras, **Greece**
14.	Titanium Dioxide Multiscale Model for Simulation of Bio-nano Interfaces **M. Ivanov** and A. Lyubartsev	**Mr. Mikhail Ivanov**, Stockholm University, **Sweden**
15.	Detecting Hepatitis B Surface Antigen Using a Novel Polycrystalline Silicon Nanowire Biosensor **C-C. Wu**, M-P. Lu, Y-F. Chang, M-R. Wang, P-T. Kuo and T-Y. Hsu	**Prof. Chi-Chang Wu**, Feng Chia University, **Taiwan**
16.	Development of Nanozyme-based Sensors for the Detection of Reactive Oxygen Species **M. David**, A. Şerban, M. Florescu and C. Bala	**Dr. Melinda David**, Transilvania University of Brasov, **Romania**
17.	Detection of non-conductive nanoparticles using Nanoparticles Imprinted Matrices (NAIMs) **L. Dery** and D. Mandler	**Mrs. Linoy Dery**, Hebrew University, **Israel**
18.	Modification of Magnetite Nanoparticles with Triazine-Based Dendrons and their Application as Drug-Transporting Systems **M. Pawlaczyk** and G. Schroeder	**Mr. Mateusz Pawlaczyk**, Adam Mickiewicz University in Poznań, **Poland**

19.	Enhancing long-term photostability of BiVO4/CdS photoanodes **H. Kmentova**, R. Yalavarthi, A. Naldoni and S. Kment	**Dr. Hana Kmentova**, Palacky University, **Czech Republic**
20.	Development of an AFM-based technique for extended write/erase endurance measurements of memristive cells V.H. Mai, V.S. Nguyen, P. Auban Senzier, C. Pasquier, … and **O. Schneegans**	**Dr. Olivier Schneegans**, GeePs Laboratory, **France**
21.	Structural and dielectric properties of CoFe2O4\LiNbO3 Bilayers **J. P. Oliveira**, B. Silva, T. Rebelo, L. Francis, J.A. Mendes and B.G. Almeida	**Mr. João Oliveira**, Univ. Minho, **Portugal**
22.	Flexible and Large-area Electrochromic Films based on PEDOT:PSS for Smart Windows **C. Park**, Y. Kim, S. Bae, M. Do, J. Min Kim and J.H.Kim	**Mr. Chanil Park**, Yonsei University, **Rep. of Korea**
23.	Overheating on aluminum metafilms by non-radiative decay of surface plasmons **D. E. Martínez-Lara**, R. González-Campuzano, J. L. Benítez and D. Mendoza	**Mr. David E. Martínez-Lara**, UNAM, **México**.
24.	Numerical Study of Graphene Oxide Capacitive Humidity Sensor with Novel Etching Configuration **S. Al Hashmi**, M. Mohammedture, J.-Y. Lu, M. Gutierrez, M. Al Teneiji	**Ms. Shamma Alhashmi**, Technology Innovation Institute- Abu Dhabi, **UAE**
25.	Design of visible-light photocatalysts for NOx removal based on LDH/BiOX nanolayered heterojunction **M.A. Oliva**, J. Ortiz Bustos, M. Cruz-Yusta, I. Pavlovic and Luis Sánchez	**Ms. Oliva Mª Angeles**, Cordoba University, **Spain**
26.	Hydrotalcite-like material for a double environmental remediation **J. Fragoso**, A. Nehdi, M. Cruz-Yusta, N. Frini-Srasra, I. Pavlovic and L. Sanchez.	**Mr. Javier Fragoso**, Cordoba University, **Spain**
27.	Challenges on the investigation of Fluorecent Probes for Heavy Metal-based Nanomaterials **J. Sanmartín-Matalobos**, P. Bermejo-Barrera, Y. Alves-Iglesias, M. Aboal-Somoza, A. M. García-Deibe and M. Fondo	**Prof. Jesus Sanmartín-Matalobos**, Santiago de Compostela University, **Spain**
28.	Metallic Nanocatalysts for Glycerol Valorization **I. Terekhina**, J. White, A. Cornell and M. Johnsson	**Mrs. Irina Terekhina**, Stockholm University, **Sweden**
29.	A Comprehensive In Vivo Study Using Drosophila melanogaster: New Insights into Mechanisms and Biological Effects of Permethrin Nanopesticides **E. Demir**, S. Kansız, M. Dogan, O. Topel, G. Akkoyunlu and M.Y. Kandur	**Prof. Esref Demir**, Antalya Bilim University, **Turkey**
30.	Interferometric Reflectance Imaging Sensor (IRIS) applied to the real-time binding detection of mycotoxin fumonisin B1 **E. Chiodi**, F. Ekiz-Kanik, M. Geib, A.M. Marn, J. Rejman, D. AnKrapp and M.S. Unlu	**Ms. Elisa Chiodi**, Boston University, **USA**
31.	Contribution to the knowledge of the Family Elateridae, Coleoptera from the Kingdom of Saudi Arabia **A. Al-Khalaf**	**Dr. Areej Al-Khalaf**, Princess Nourah bint Abdulrahman University, **Saudi Arabia**
32.	Multifunctional Nanocoatings to Overcome Contact Lenses Associated Conditions and Discomforts **S.A. Khan** and C.S. Lee	**Mr. Shakeel Khan**, City University of Hong Kong, **Hong Kong**
33.	Studies on the possibility of using modified titanium oxide as a poten-tial drug carrier **O. Długosz**, J. Pulit-Prociak and M. Banach	**Dr. Olga Dlugosz**, Cracow University of Technology, **Poland**
34.	Efficient photodegradation of dye-polluted water by a high-flow rate functionalized microreactor **N. Martin**, V. Lacour, C. Perrault, E. Roy and Y. Leprince-Wang	**Dr. Nathan Martin**, Université Paris-Est-Marne-la-Vallée, **France**
35	Supercritical Fluid Extraction and Pressurized Liquid Extraction Processes Applied to EPA-rich Polar Lipid Recovery from the Microalga Nannochloropsis sp. **MJ. Jiménez-Callejón**, A. Robles-Medina, MD. Macías-Sánchez, PA. González-Moreno, E. Na-varro-López, L. Esteban-Cerdán and E. Molina-Grima	**Prof. María José Jiménez**, University of Almería, **Spain**

36	Time evolution of Molecular Binding in Mechanically controlled Break-Junctions **M. Lokamani**, F. Günther, F. Kilibarda, J. Kelling, S. Gemming and A. Erbe	**Mr. Mani Lokamani**, Helmholtz-Zentrum Dresden-Rossendorf, **Germany**
37	Process for the synthesis of nanostructures based on two-dimensional materials under concentrated solar irradiation **T.Barbe**, F.Bataille, G.Flamant, E.Nadal and A.Vossier	**Mr. Timothee Barbe**, PROMES-CNRS, **France**
38	Characterization of protein-utilizing group in anaerobic fermenters **Z.Deng**, H. Spanjers and J. B. van Lier	**Ms. Zhe Deng**, Delft University of Technology, **The Netherlands**

Nanotech France Session I.A

Exploiting Functional Materials for a Better Life

Rodrigo Martins[1,2], Suman Nandy[1], and Elvira Fortunato[1,2]

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[2] AlmaScience, Campus de Caparica 2829-516 Caparica, Portugal

Abstract:
Today science is essential to enable comfort and welfare, as well as prosperity to regions and countries. This implies fostering the creativity of scientists and consequent innovations to support the current societal challenges. In this respect, advanced materials offer a variety of solutions that are based on the idea that "Materials are everywhere even in our body!". Within these solutions, it is vital to consider the reuse of residues, recycling and circularity to serve a Green Agenda and bring an eco-sustainable environment, as we do not have a planet B as alternative solution! The idea is to SEE the world through, Sustainability-Environment-Economy challenges. In fact, the role of advanced materials is to foster several economic sectors, by exploiting materials on their multiple latitudes to provide outstanding structural and functional applications of materials, particularly by understanding the nanoscale, as this is the scale by which the digital, bio and physical worlds can communicate and interact.

In this presentation, we aim to present data on functional materials, able to be processed at low temperatures and to impact in the key sectors of electronics, energy, health and packaging, namely when exploited their performances at a nanoscale.

A sustainable alternative to flexible electronics based on metal oxide materials

E. Fortunato, P. Barquinha, E. Carlos, R. Branquinho, R. Martins

CENIMAT/i3N Departamento de Ciência dos Materiais, Faculdade de Ciências e Tecnologia (FCT), Universidade NOVA de Lisboa (UNL), and CEMOP/UNINOVA, 2829-516 Caparica, Portugal

Abstract:

Metal oxide semiconductors are a good example as a success story in the area of thin film electronics, since it took less than 10 years after the discovery until the commercialization of the first products mainly in the area of displays. The main advantages of these materials are the low temperature processability, the high mobility and the uniformity over large areas, since they present an amorphous structure.

Nevertheless to decrease costs associated to electronic devices a strategy is using cheap and abundant materials in conjunction with low cost fabrication methods, associated to an overall increase of electrical performance. This is why metal oxide semiconductors are the key materials since they are chemically stable, mostly non-toxic and abundant materials, often manufactured by low cost methods, under ambient conditions. Consequently, devices made of metal oxides are inexpensive, very stable and environmentally safe, the 3 most important requirements for electronics.

Despite being explored for more than a century for electronic applications, from the initial works of Badeker in 1907 with CdO to the cutting edge IGZO available these days in active matrix backplanes of flat panel displays, oxides still present an exceptional and innovative combination of properties not achievable by any other material class. In fact, they are true multifunctional materials, being able to exhibit optical transparency, conducting / semiconducting / insulating behaviour, piezoelectricity and catalytic or self-cleaning properties among many others.

In this presentation we will review some of the most promising new technologies based on oxide conductors, semiconductors, dielectrics as well as electrochromic devices either in the form of nano-films or nanoparticles, and we will summarize the major milestones already achieved with this emerging and very promising technology focused on the work developed in our laboratory [1,2].

By using these materials and technologies we are contributing to the evolution of environmentally conscious electronics that is able to add new electronic functionalities onto surfaces, which currently are not used in this manner.

Keywords: metal oxides; thin film transistors; flexible electronics;

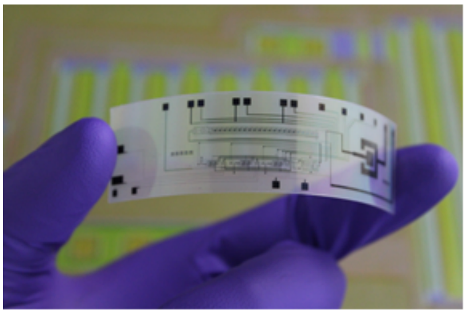

Figure 1: Example of flexible electronics based on metal oxide devices.

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1. E. Fortunato, P. Barquinha, and R. Martins, "Oxide Semiconductor Thin-Film Transistors: A Review of Recent Advances," Advanced Materials, vol. 24, pp. 2945-2986, Jun 12 2012.
2. P. Barquinha, R. Martins, L. Pereira and E. Fortunato, Transparent Oxide Electronics: From Materials to Devices. West Sussex: Wiley & Sons (March 2012). ISBN 9780470683736.

Trends in nanometrology using smart sensing with electron microscopes

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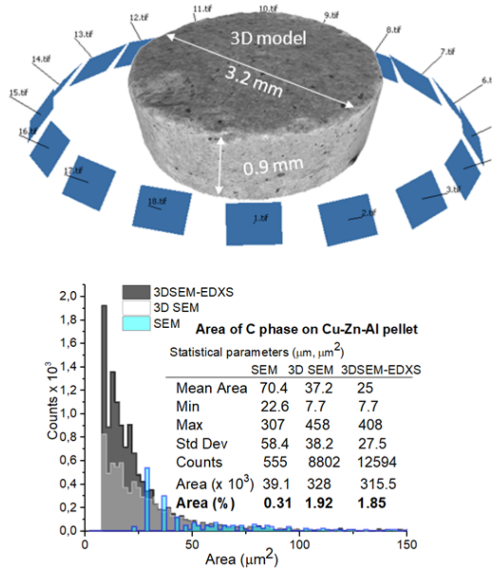
[1] University of Cádiz, Department of Physics of Condensed Matter, 11510 Puerto Real, Spain

Abstract:

There is a growing prevalence in materials characterization of datasets that are much too large for human-directed detailed analysis of individual measurements. Moreover, this trend will continue to grow in the future. For instance, this is the case within the context of the characterization of materials using electron microscopy (EM) where there is growing interest for developing systematic ways to make measurements (nanometrology) from the raw data with real-time analytics and visualization. Here, we discuss advances on the implementation of data compression with edge-computing for increasing the efficiency of real-time nanometrology in electron microscopy.

Another area of development in EM is the access of information about surfaces in three-dimensions (3D). Among several techniques multiview photogrammetry (MVP) allows the reconstruction of high-resolution 3D models using an scanning electron microscope. Although the principles of the technique, i.e. stereo photogrammetry are old, recent developments in hardware and software permits its application to build complex 3D models with any SEM and using personal computers. The 3D models can be used to measure geometrical properties and mapping chemical distributions with greater accuracy. In this talk we discuss also the workflow for 3D SEM, and we show applications of the technique to study different materials from the nano- to the millimeter- scales including, (1) an study of adhesion wear, the mechanical properties of a nanoscale, the surface roughness of patterned samples or the physico-chemical characterization of the surface of commercial water gas shift catalyst bodies.

Keywords: electron microscopy, photogrammetry, sensors



Statistical parameters (μm, μm^2)

	SEM	3D SEM	3DSEM-EDXS
Mean Area	70.4	37.2	25
Min	22.6	7.7	7.7
Max	307	458	408
Std Dev	58.4	38.2	27.5
Counts	555	8802	12594
Area (x 10^3)	39.1	328	315.5
Area (%)	**0.31**	**1.92**	**1.85**

Figure 1: Top, 3D model of a catalytic pellet of Cu-Zn-Al. Bottom, distributions and several statistical parameters of the areas of carbon particles measured from data obtained using SEM, 3D SEM and 3DSEM-EDXS.

References:

1. Gontard, L.C. *et al.*, Cellular-Neural-Network Focal-Plane Processor as Pre-Processor for ConvNet Inference. 2020 *IEEE International Symposium on Circuits and Systems* (ISCAS), Sevilla, 2020, 1-5.
2. Gontard, L.C., Batista, M., Salguero, J., Calvino, J.J. (2018), Three-dimensional chemical mapping using non-destructive SEM and photogrammetry, *Sci. Rep.*, 8(1), 1-10.
3. Gontard, L.C., Cauqui, M.Á., Yeste, M.P., Ozkaya, D., Calvino, J.J. (2019), Accurate 3D Characterization of Catalytic Bodies Surface by Scanning Electron Microscopy, *ChemCatChem*, 11(14), 3171-3177.

Nanotech France
Session I.B: Nanomaterials Fabrication/ Synthesis/ Charecterisation

Surface engineering of nanomaterials for water treatment

A.L. Daniel-da-Silva [1*]

[1] CICECO-Aveiro Institute of Materials and Chemistry Department, University of Aveiro
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Abstract:

Clean water is of crucial importance for global health and economic development. A wide range of emerging pollutants are frequently detected in drinking water sources, treatment plant effluents and natural waters at levels that may jeopardize public or ecosystem health.[1] These pollutants include pesticides and contaminants of emerging concern, such as pharmaceuticals and personal care products that disrupt endocrine systems or cause other effects. These facts highlight the need for technological innovation in the development of effective water treatments.

Nanotechnology has provided new opportunities to enhance the efficiency of water remediation treatments and wastewater reuse through the development of surface-engineered nanomaterials for the adsorption of pollutants.[2,3] Nanomaterials possess increased specific surface area and unique surface properties such as surface chemistry and wettability of relevance for water treatment and contaminated site remediation.[4] Ideally, a sorbent for water remediation should fulfil the following requirements: specificity to the target pollutants, high adsorptive performance, rapid adsorption, cost-effective, environmentally non-toxic, reusable and easy separation from treated water. Low toxicity and easy magnetic separation can be met by a simple combination of biopolymers with magnetic iron oxide nanocrystals. However, a rational design of the surface of the nanocrystals is needed to attain specificity, high adsorption capacity and reusability. Herein, novel chemical strategies for the surface modification of nanoparticles are discussed through several examples of systems developed for specific applications in water remediation. The focus will be given to the rational design of the surface of magnetic nanomaterials with biopolymers, aiming the development of advanced nanosorbents with high adsorptive performance and reusability.[5-7]

Keywords: magnetic nanoparticles; biosorbents; polysaccharides; surface modification; emerging contaminants; adsorption

References:

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2. Alvarez, P. J. J.; Chan, C. K.; Elimelech, M.; Halas, N. J.; Villagrán, D. (2018) *Nature Nanotechnology*, 13, 634.
3. Jassby, D.; Tzahi, Y.; Cath, T. Y.; Buisson, H. (2018) *Nature Nanotechnology* 13, 670.
4. Daniel-da-Silva, A.L.; Trindade, T. (2021) Applications of Colloidal Nanocrystals, ch 6, In *Surface Chemistry of Colloidal Nanocrystals* 209-257.
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Challenges on 2D materials in PVDF porous membranes designed to water desalination

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Abstract:

Water scarcity together with pollution levels in water represents a real risk for human health and environment. Ambitious solutions based on sustainable technologies are imperative for the management of natural water resources and environment protection. This work discloses the key role of 2D materials in two green membrane technologies designed to water desalination. 2D materials engineered membranes are fabricated and used as functional interfaces in membrane distillation (MD) and membrane crystallization (MCr) devices. Larger and better quality production of freshwater is achieved, while salt crystals are recovered according to more uniform size and shape distributions. Energy saving operations are also accomplished due to reduced heat dissipation during water distillation. Enhanced resistance to undesired fouling events is further proved. Experimental evidences suggest an involvement of 2D nanofillers in water transport. Chemisorption mechanisms at the vacancies of exfoliated few layers materials are envisaged to accelerate water diffusion through the membranes, thus promoting higher fluxes as well as quicker nucleation and growth rate of crystals under supersaturation conditions. Comparative analyses provide new insights about the opportunity to confine 2D materials in polymeric membranes in order to well address water desalination processes. These achievements can be regarded as a prelude to the development of new-concept nanocomposite membranes for fruitful water desalination through environment-friendly approaches. 2D materials-engineered membranes show to be promising to travel successfully on the path to scaled up and eco-sustainable membrane distillation and membrane crystallization processes in full agreement with natural resources and biodiversity concepts.

Keywords: Water desalination, nanoporous hydrophobic membranes, 2D materials-enabled membranes, assisted water diffusion, crystal nucleation and growth Membrane Distillation, Membrane Crystallization, green water purification.

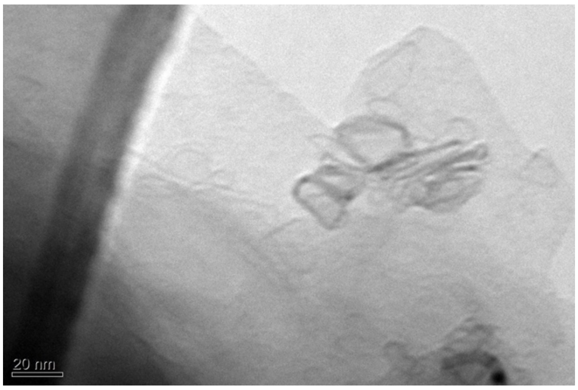

Figure 1: Figure illustrating TEM picture of exfoliated bismuth telluride crystals confined in polymeric membranes and designed to water desalination purpose.

Acknowledgements

We acknowledge financial grant from 'the Italian Ministry of Foreign Affairs and International Cooperation' within the framework of the Great Relevance International Project Italy (MAECI)-China (NSFC) 2018-2021 - New Materials, with particular reference to Two-dimensional systems and Graphene (2DMEMPUR)

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Scalable and sustainable synthesis to produce iron oxide nanoparticles

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Abstract:

The opportunity to produce nanomaterials on industrial scale for widespread applications represents today a real challenge. Among nanomaterials, iron oxide nanoparticles (IONPs) are very promising thanks to their flexibility in several application fields. This presentation concerns a patented, eco-friendly and scalable method to synthesize IONPs dispersed in water. [1, 2] The method, using an ion exchange process, allows producing various iron oxides or hydroxide nanoparticles (NPs) in one-step with cheap or renewable reagents. In particular, an anionic resin is mixed with an aqueous solution of iron(II) and iron(III) salts, maintaining them under stirring up to 10 minutes, working at room temperature and ambient pressure. After the ion exchange, the resin is separated from the synthetized NPs through a simple sieving procedure, and then it can be regenerated. The obtained iron NPs can also be used as precursors to produce other iron oxides NPs with different aging or calcination procedures. The main applicable types of iron oxide/oxyhydroxide NPs are obtained: ferrihydrite, δ-FeOOH, magnetite, hematite, and maghemite, with a high purity, small particles dimensions (<30 nm) and high specific surface area, with yields of production >90%. Structural and morphological features of the obtained NPs are investigated by XRD, TEM, SEM and BET measurements. [3]

In particular, 2-line ferrihydrite nanoparticles result monodispersed with dimensions of about 2 nm and a measured BET surface area of 420 m^2/g, with an isotherm typical of microporous materials. As concerns the hematite nanoparticles, they have hexagonal plate-like morphologies, with the largest dimension of about 30 nm and a measured BET surface area 58 m^2/g. Moreover, the magnetite NPs are cubic and monodispersed, having dimensions of about 6 nm and a BET surface area of 169 m^2/g with an isotherm typical of mesoporous materials.

Keywords: nanoparticles synthesis; ion exchange process; iron oxide nanoparticles; ferrihydrite NPs; hematite NPs; magnetite NPs; XRD; TEM; SEM; BET.

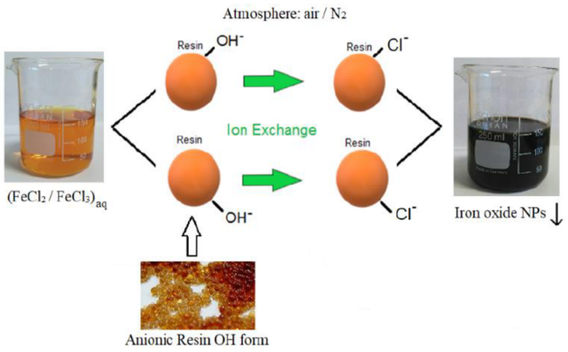

Figure 1: Schematic illustration of the ion exchange synthesis process, starting from an aqueous solution of iron chlorides mixed with a suitable amount of anionic resin (OH^- form), leading to the direct production of iron oxide nanoparticles in 10 minutes at root temperature and ambient pressure.

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Sustainable and eco-compatible nanolime based treatments in aqueous medium for the conservation of cultural heritage

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Abstract:
The use of nanotechnology is gaining an increasingly attention particularly in the field of Cultural Heritage conservation but, at now, nanomaterials are long way from being routine treatments due to their production processes or to the fact that nanoparticles (NPs) pose concerns regarding human health and environmental risks, also in relation to their dispersing medium.

This work aimed to present our cost-effective, sustainable and patented synthetic procedure [1], allowing us to produce calcium hydroxide NPs (also called nanolime), Fig.1, directly in aqueous dispersion, overcoming the main limitations of synthesis processes found in literature and giving us the possibility to scale up the NPs production from laboratory to an industrial scale. Moreover, the use of water as dispersing medium allowed paving the way of extensive usage of nanolime in cultural heritage, such as on architectural surfaces treatments. This eco-friendly and time-energy saving route is based on an ion exchange process, operates at room temperature, starts from cheap or renewable reactants, without intermediate purification procedures, so reducing the time of synthesis and greatly improving the yield of production. The produced NPs dispersions show a high reactivity, assuring a complete carbonation process in few hours and also at moderate moisture conditions [2]. The aqueous nanolime-based treatments are successfully employed for the conservation of Agrigento's biocalcarenites and they were tested, for the first time, in an on-situ application for the consolidation of an historic mortar of a medieval palace [3-4]. In both cases, the treatments show a good consolidation effectiveness, with a reduction of the removed material after treatment > 80% together with an improvement in the drilling resistance, respect to the untreated substrate, demonstrating a penetration more than 10 mm from the surface. Moreover, no chromatic alteration of the surfaces and safety health and environmental conditions are guaranteed too.

Keywords: Calcium hydroxide nanoparticles; Aqueous suspensions; Sustainable and innovative treatments; Agrigento's biocalcarenites; Conservation of historical mortar

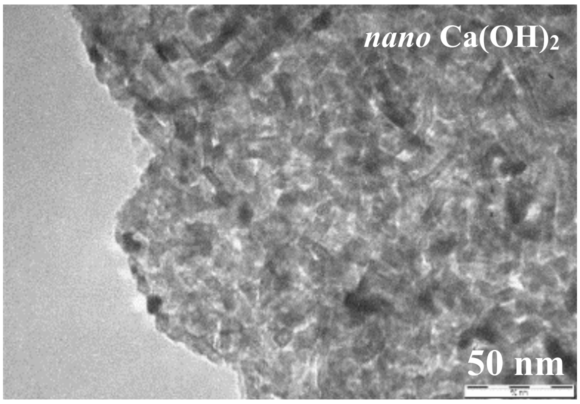

Figure 1: TEM image of nanolime particles, in aqueous suspension, synthesized by means of our innovative and sustainable synthetic route. The nanolime particles appear constituted by a self-assembly of primary nanoparticles, with dimensions less than 10nm.

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Design, synthesis and characterization of polystyrene nanoparticles doped with lanthanide complexes for photoacoustic and near-infrared luminescence imaging

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Abstract:

Several types of nanomaterials for use in biological imaging have generated a high level of excitement in the last few years. Among different types of novel imaging techniques, near-infrared luminescence and photoacoustic (optoacoustic) imaging have attracted increasing attention. Each technique possesses specific advantages: near-infrared (NIR) luminescence is extremely sensitive and allows the acquisition of images with high resolution at the cellular level while photoacoustic imaging provides higher detection depth. Both techniques require specific imaging agents which exhibit large molar absorption coefficients and can be excited with a light, the wavelength of which corresponds to the transparency window of biological tissues.

In this work, we are creating combined imaging agents based on 100 nm polystyrene nanoparticles loaded with lanthanide complexes that satisfy the requirements of both photoacoustic and NIR luminescence imaging techniques.

Lanthanide ions possess unique optical properties: they exhibit line-like emission bands with wavelength positions in the visible and in the NIR ranges that are not affected by experimental conditions, large energy difference between excitation and emission bands and long luminescence lifetimes, which makes them excellent candidates for luminescence imaging. As a drawback, their emission intensities are limited by small absorption coefficients due to the forbidden nature of most of f-f electronic transitions.

To overcome this limitation, organic chromophores with high absorption coefficients are used as sensitizers by absorbing the energy of the excitation light and transferring it to the accepting levels of the lanthanide ion. In addition, these chromophores possess a large number of vibrations that can be used for photoacoustic detection.

In this work, Yb^{3+}complexes formed with β-diketonate ligands connected to NIR absorbing chromophores were synthesized and characterized. Their photophysical properties were extensively investigated. Synthesized lanthanide complexes were encapsulated inside 100 nm polystyrene nanoparticles to allow their uses in biological conditions. Resulting polystyrene nanoparticles were fully characterized, their size, polydispersity and stability were investigated. The amount of the loaded lanthanide complexes was determined. It was observed that under excitation in the biological window, the polystyrene nanoparticles loaded with the lanthanide complexes provide both NIR emission and photoacoustic signals (Figure 1), which makes them promising candidates as a new generation of bimodal imaging agents.

Keywords: lanthanides, complexes, polystyrene nanoparticles, photoacoustic imaging, near-infrared luminescence imaging.

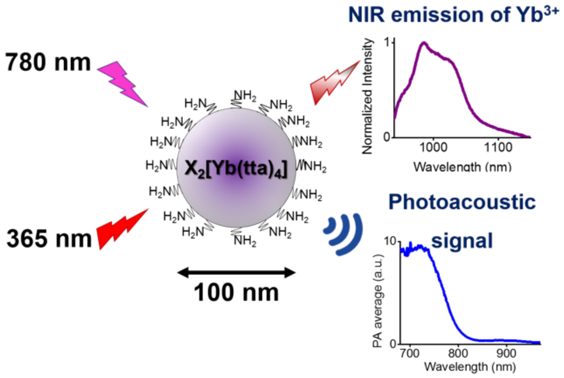

Figure 1: Figure illustrating the possibility of ytterbium-containing polystyrene nanoparticles to exhibit the photoacoustic and the NIR luminescence signal.

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Tunable red-to-white luminescence of strontium vanadate

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Abstract

Novel materials with advanced optical properties are highly demanded with the rapid development of light technology. Vanadate materials doped with lanthanide ions are widely researched because of their excellent luminescent properties. The most frequently studied are orthovanadates i.e. the YVO_4: Eu^{3+} known as red phosphors, and the YVO_4: Yb^{3+}, Er^{3+} upconverting green light source [1]. Furthermore, complex materials containing vanadates also exhibit interesting luminescence properties [2].

The $Sr_3(VO_4)_2$: Eu^{3+} luminophor exhibits bimodal red and white luminescence due to the use of excitation with different wavelength (λ). After self-activation by charge transfer from the oxygen *2p* orbitals to the *3d* orbitals of vanadium ions, these materials show altered white luminescence after UV excitation [3]. This feature can be also used as a charge transfer band for transmission energy to Eu^{3+} dopant ions to observe characteristics for the Eu^{3+} ion red emission bands.

Here, various approaches to the synthesis of $Sr_3(VO_4)_2$: Eu^{3+} by the Pechini method were explored. Crystal structure differences were examined by XRD and morphology was investigated by SEM. The luminescence properties i.e. emission and excitation spectra, etc. were investigated with spectrofluorimetry.

Tuning of emission color was observed with a different approach in the sol-gel synthesis process (Fig.1). The results indicate a changed crystal structure and radical changes in the luminescence properties of obtained materials when the synthesis approach was changed.

Keywords: lanthanides, vanadates, luminescence, tunable luminescence, inorganic nanomaterials, spectroscopy, sol-gel synthesis, europium, strontium vanadates, charge transfer,

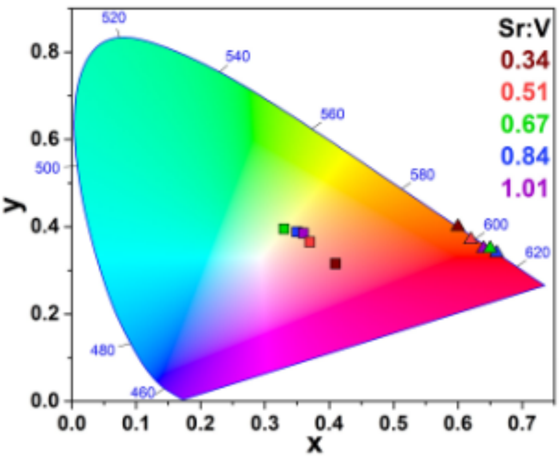

Figure 1: CIE diagram for strontium vanadate materials for excitation at λ_{ex}=393nm (triangles), and λ_{ex}=345nm (squares).

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Acknowledgment

The work was supported by grant no. POWR.03.02.00-00-I023/17 co-financed by the European Union through the European Social Fund under the Operational Program Knowledge Education Development, and by the Polish National Science Centre (UMO-2018/31/N/ST500636).

Study of Cu coordination core in copper complexes grafted onto Au nanorods

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Abstract:

Copper coordination compounds have been developed as a promising alternative to the classic anticancer metallodrugs [1].

In our quest for suitable organic ligands that exhibit a remarkable cytotoxic activity we focused our attention on the synthesis of Cu(II)-complexes of bis(azol-1-yl)acetates and related esters or amides [2]. However, since these compounds have low solubility in aqueous medium, it is necessary to design a strategic approach allowing for drug delivery. In our recent works we are exploring the possibility to conjugate the copper complexes with hydrophilic gold nanoparticles (AuNPs), to improve their solubility and stability in water, increasing their bioavailability. The preliminary studies confirmed the success of the method [3,4].

An accurate study of the Cu coordination core is a mandatory step to understand the grafting to Au-NPs and the Au-NP/Cu-complexes stability in order to individuate the suitable procedures for controlled drug release.

In this work the local atomic structure and coordination chemistry around Cu and Au atoms in different Au-NP/Cu-complexes [5] has been probed by X-ray absorption fine structure (XAFS). The data provide a deep insight on the interaction between Au-NP and Cu(II)-complexes sheding light on the mechanisms for drug loading/release.

Such information is relevant to reliably understand the activity of this novel drug delivery systems representing a step forward in developing specific metal-based anticancer drugs.

Keywords: Gold Nanoparticles, copper complexes, local coordination chemistry, anticancer drugs, drug delivery system.

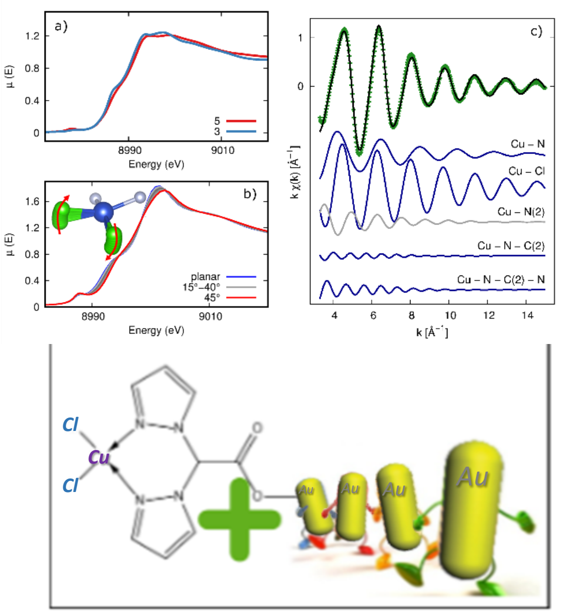

Figure 1: Top panel: Results of the Cu K-edge XAFS data analysis. Bottom panel: pictorial example of a Cu(II) complex conjugated with Au-nanorods.

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Detection of organophosphorous compounds with nanostructured microcantilever-based sensors

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Abstract:
Microcantilever-based sensors are promising sensitive detection systems despite their low surface area for the capture of the analytes in vapor phase. In order to enhance the detection performance of a commercial optical microcantilever, we report a strategy that increases the surface area of the microcantilever for sensing of analytes in vapor phase. Different nanostructurated metal oxides and particularly titanium dioxide nanowires (TiO_2-NWs) were synthesized on the surface of the microcantilevers by hydrothermal method or soft chemistry. Effects of the synthesis conditions on the nanostructures were studied on centimetric silicon substrates. Subsequently, the synthesis procedure was transferred onto a microcantilever. This transfer requires specific synthesis modifications in order to obtain a homogeneous and stable nanostructuring on the front side of the microcantilever. Studies on the effects of nanostructures on the physical properties as the resonance frequency of microcantilevers were carried out. These nanostructured microcantilevers were designed for the detection of vapors of Chemical Warfare Agents (CWAs), specifically nerve agents. Dynamic mode detection measurements were evaluated with dimethylmethylphosphonate (DMMP), simulating sarin (GB). The increase of the surface area on microcantilevers shows a gain in sensitivity compared to unmodified microcantilevers. The adsorption of DMMP is mainly driven by hydrogen-bond formation to hydroxyl groups on the surface of the metal oxides. Nanostructured microcantilevers highlight interesting perspectives to enhance easily the sensing performances of organophosphorous compounds in vapor phase.

Keywords: Nanostructured microcantilever-based sensors, organosphosphorous compounds, chemical warfare agents, TiO_2 nanostructures

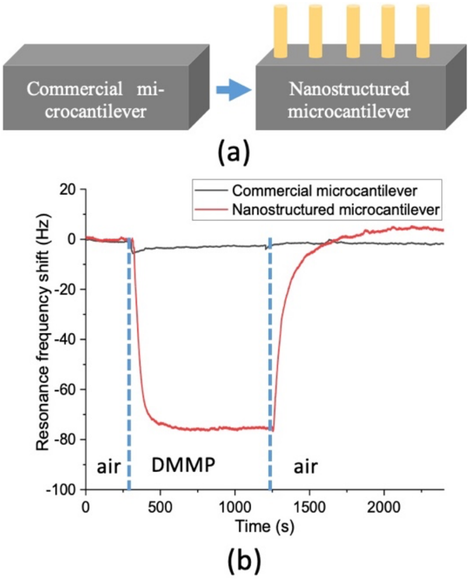

Figure 1: (a) figure illustrating the modifications brought with the nanostructuring of the microcantilever and (b) diagram showing the response at the same concentration in DMMP before nanostructuring (black curve) and after nanostructuring (red curve) of the commercial microcantilever.

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Highly reproducible gram-scale CdSe/CdS giant-shelled nanocrystal synthesis with tunable particle geometry

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Abstract:

We developed a synthesis for CdSe/CdS giant-shelled nanocrystals with adjustable diameter from 8-20 nm, based on Bawendi [1]. By analytical in situ characterization and systematic parameter variation, we got the key knowledge of the growth mechanism.

Further, we managed to upscale the synthesis to the gram-scale with focus on reproducibility. To achieve this, it was necessary to control the precursor flow rates precisely over time with an automatic set up.

The resulting particles show a very high crystallinity, quantum yields >90%, red emission at 625 nm and an adjustable size (8-20 nm).

Furthermore, by changing only one parameter the shell geometry can be easily tuned from a sphere to a flat hexagon (plate), see figure. Those plates have the property to align with the crystallographic c-axis perpendicular to the substrate. Aligned 2D materials show interesting properties, like a circular polarized light emission. Like the spherical giant-shelled nanocrystals this plate synthesis is highly reproducible, too. Both materials show very high absorption below 480 nm, high quantum yields and high photo stability. This makes them ideal for display applications.

Keywords: Nanoparticle, CdSe/CdS, giant shell, colloidal synthesis, quantum materials, scale up, optoelectronic applications (LED), biomedical tag, luminescent solar concentrator

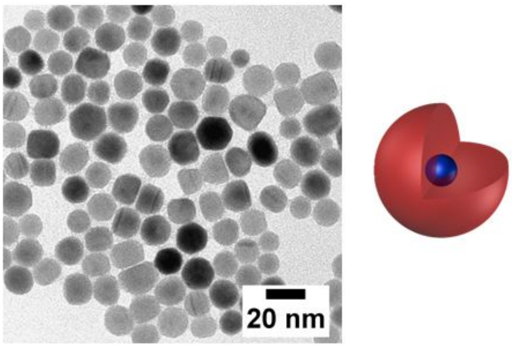

Figure 1: The left transmission electron microscope image shows these spherical CdSe/CdS giant-shelled particles. The right transmission electron microscope image shows the CdSe/CdS plates based on the same spherical CdSe cores.

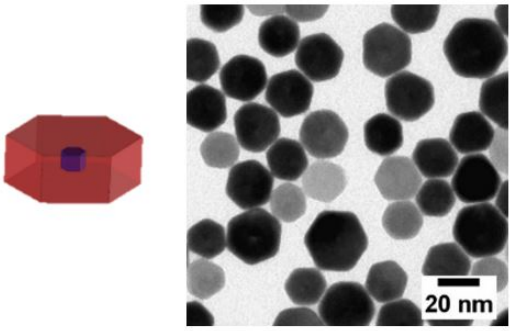

Figure 2: The left transmission electron microscope image shows these spherical CdSe/CdS giant-shelled particles. The right transmission electron microscope image shows the CdSe/CdS plates based on the same spherical CdSe cores.

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Nanofibrillar Green Composites of Polylactide/Polyamide Produced in Situ Due to Shear Induced Crystallization

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Abstract:

With extremely growing awareness of environmental issues, the demand for plastics is being shifted from conventional materials to renewable and natural polymers. Two different approaches are often employed for production of green polymer-based materials. The first one is blending of two biopolymers with or without using natural plasticizers or compatibilizers as a third component. The second approach deals with adding natural polymers in the form of fibers or particles into biopolymer matrix. In both cases the properties of the obtained blends correspond to the so-called mixture rule, when they are the arithmetic mean of the properties of each of the components. Recently in-situ (one-step) and ex-situ (multi-step) nanofibrillar reinforced green polymer-polymer composites (NFCs) has gained a lot of interest because this type of material provides a way to tailor the properties of the resultant blends so that it combines the best properties of both its constituent components. The key role in achieving this result is played by specifically designed morphology of these blending systems such as entangled nanofibers, shish-kebab structures, etc [1, 2].

Current research deals with the development of a new method of manufacturing of green NFCs when the final material combines the best properties of both components. It is based on the simultaneous realization of orientation and crystallization of polymer fibers directly at the stage of extrusion in a single step by setting high shear strain and shear rate, which causes nodular to fibrillar transition and forces crystallization of a polymer at a higher temperature without a succeeding cooling.

This possibility was demonstrated by using two entirely bio-sourced polymers: polylactide (PLA) and biopolyamide (PA) as components.The link between the morphology of NFCs and the rheological properties of used polymers has been investigated. It has been established that suitable rheological conditions for stimulating deformation and extension of droplets into fibers are the viscosity ratio (the ratio of the viscosity of the matrix to the viscosity of the dispersed phase) and elasticity ratio (the ratio between the Weissenberg number of the droplet phase and matrix) lower than unity. A chain extender agent with multiple epoxy function (Joncryl ADR 4400, Basf, Germany) was used in order to increase the viscosity and elasticity of PLA matrix. An increase in shear rate also contributes to a decrease in elasticity ratio and accordingly, to the formation of a more favorable PA fibrillar morphology. It has been shown that there is a critical shear rate at which the shear inducing crystallization may solidify PA nanofibers without subsequent cooling. Shearing of PA increased non-isothermal crystallization temperature by 40 ^{0}C and decreased the temperature range in which the transition from a molten state to a crystallized one occurs by 10 ^{0}C. The formation of a network of fibrils contributes to the simultaneous increase in the rigidity and strength of the NFCs.

Keywords: green polymer-polymer nanocomposites, shear induced crystallization, in situ fibrillation, rheological and mechanical properties.

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Multi-functional Natural Fiber Composites for Shear Loading

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Abstract:

An experimental investigation is conducted to study the effect of shear loading on the mechanical and electrical response of multi-wall carbon nanotube (MWCNT)/carbon fiber (CF) interlayer reinforced jute/epoxy composites. Four factors such as weight fraction of MWCNTs (0.1 and 0.025 wt%), carbon-flock fiber length (150 and 350 µm), flock density (500, 1000, 1500 and 2000 fibers/mm2), and jute fiber orientation (0-0-0-0 and 0-90-0-90) are considered. The MWCNTs are embedded in the epoxy matrix using combination of sonication and shear mixing. The CFs are positioned vertically on the jute fiber laminate-layers by the UMass Dartmouth patented "wet flocking" technique. The embedded MWCNTs and reinforced CFs between the laminate plys generate a three-dimensional electrical conductive network in the composite (Fig 1). The resistance change of the composite associated with the inter-laminar shear is investigated by the four-circumferential ring probes (FCRP) technique. The effect of above listed factors on the electro-mechanical response of the composites under shear loading is studied.

Overall, the hybrd natural fiber composites presented in this work are truly multi-functional because CF reinforcement between the laminate-layers not only improves the interlaminar shear strength, but also provides sensible conductive network within the composite to detect damage under mechanical loading conditions. CF flocking parameters such as flock density and fiber length provide a good design space in developing materials for damage sensing in structural load bearing applications.

Keywords: Nanocomoosites, Multi-wall Carbon Nanotube (MWCNT). Four-circumferential Ring Probes (FCRP)

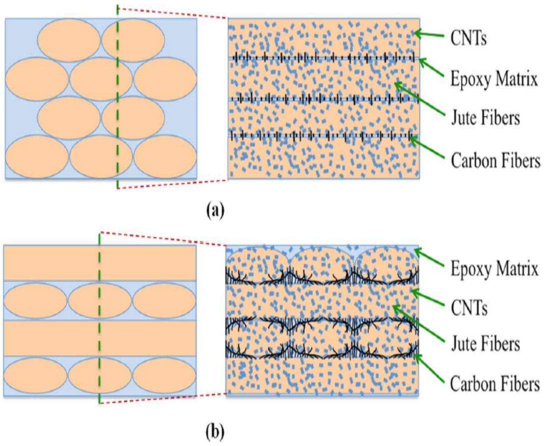

Figure 1: Conductive network generated between CNTs and carbon fibers of laminate orientations with a cross-sectional view of highest path of resistance for (a) (0-0-0-0)T, and (b) (0-90-0-90)T.

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The effect of sintering temperature on the electro physical properties of Silicon-polymer based composite Varistors

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Abstract:

Nowadays electronic Silicon–polymer composite varistors were prepared through hot pressing at a pressure of 60 MPa and different temperatures and their current-voltage characteristics were investigated. The results show that these varistors can be used to protect circuits from 200 V up to 500 V overvoltage. In addition, it is found that the varistor breakdown voltage and its nonlinearity coefficient as well as its impurity band gap increase by increasing sintering temperature while the corresponding potential barrier height decreases. Due to the presence of polyethylene in the Silicon–polymer composite varistors, fluctuation in breakdown voltage, nonlinearity coefficient, leakage current, potential barrier height, and the optical gap has been observed. Finally, the sintering temperature effect on leakage current, breakdown voltage, and nonlinear coefficient was both investigated and analyzed using scanning electron microscopy and XRD patterns. The results show that 130 C is the optimized temperature to produce Silicon–polymer composite varistors.

Keywords: varistor, Composite, Silicon, Poly Aniline, polyethylene, Non-linear coefficient, Voltage, Current and Temperature.

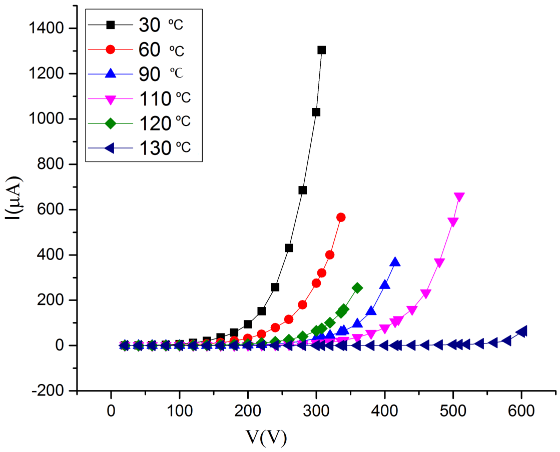

Figure 1: current–voltage characteristics of Silicon-polymer composites which sintered at different temperatures, i.e., 30 ^{o}C, 60 ^{o}C, 90 ^{o}C, 110 ^{o}C, 120 ^{o}C, 130 ^{o}C.

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The effect of sintering pressure on the electro physical properties of Silicon-polyaniline–polyethylene composite Varistors

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Abstract:

The rapid development of electronic equipment attracts the attention of various fields of science such as particle physics, medicine, imaging, etc. One of the outcomes of this development is sensor technology known as an essential element in medical imaging. As an example, Silicon Photomultiplier (SiPM) plays a significant role in this field. The main outcome of combining different techniques to enhance the performance of SiPM leads to circuits that are highly sensitive and accurate. The cost of such accuracy is their sensitivity to any voltage fluctuation that can have serious damage to the sensor. In this research, we are introducing a novel method of varistor construction with various functionality performance based on nanomaterials, that can enhance the protection of critical circuits against voltage fluctuation.

Silicon–polyaniline–polyethylene composite varistors were prepared through hot pressing methods in a matrix with 10 mm diameter at a temperature of 130 C and different pressures and their current-voltage characteristics were investigated. Results show that these varistors can be used to protect circuits from 240 V up to 520 V over-voltage. In addition, the varistor breakdown voltage and the corresponding barrier height increase by increasing sintering pressure while the leakage current decreases. Since by increasing sintering pressure to 60 MPa, the non-linearity coefficient will increase but by increasing the pressure more than 60 MPa, the non-linearity coefficient goes down. Thus 60 MPa is optimized pressure for production Si–polyaniline–polyethylene composite varistors. The analysis of composite samples by scanning electron microscopy and XRD patterns are presented.

Keywords: varistor, SiPM, Composite, Silicon, Poly Aniline, polyethylene, Non-linear coefficient, Voltage, Current and pressure.

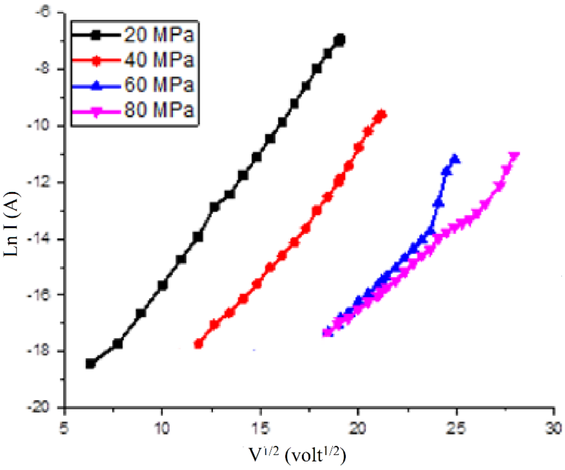

Figure 1: (Ln I - □$V^{1/2}$) diagram for Silicon-polyaniline–polyethylene composites which sintered at different pressures, i.e., 20 MPa, 40 MPa, 60 MPa, 80 MPa.

References:

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MBE Growth and NC-AFM/KPFM characterization of 2 D materials under UHV environnement : graphene and silicene.

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Abstract:

Recently, the two dimensional (2D) material is gaining increasing research interest for applications in nanoelectronics and spintronics, like graphene, a one-atom thick carbon sheet with honeycomb sp^2 configuration. Graphene is also a good candidate for substrates used in the growth of new 2D materials like silicene : the silicon-based version of graphene. Such 2D materials exhibit interesting phenomena as : quantum Hall effect, superconductivity and hight thermal conductivity.

In my proposal presentation, we present our work on how to characterize, based on the height and the surface potential, and using coupled nc-AFM and KPFM microscopy techniques, different types of graphene, that can possibility be the substrate for our silicene growth : Zero-layer graphene (**ZLG**) (**2.62 Å, 4.09 ± 0.05 eV**) , Quasi free standing monolayer graphene (**QFMLG**) (**4.09 Å, 4.63 ± 0.05 eV**) and bilayer graphene (**BLG**)(**6.86 ± 0.14Å**)[1] (Fig.1).

The second part of this work is the silicon growth on the graphene/6H-SiC (0001) substrate in a MBE chamber under UHV condition. The growth was governed by diffusion-limited aggregation (DLA). We found that a flower-like silicon were nucleated on graphene and SiC/graphene edges (Fig.2) at a room temperature with a fractal shape. The size of the island became larger and maintained their flower-like form when we increase the Si time deposition rate.

We can clearly observe with nc-afm microscopy that the flower-like island were not monoatomic (**1.2 nm**) and thus, the 2D silicene sheet can not grow on graphene or 6H-SiC(0001) as predicted by DFT calculations[2] .

Keywords: NC-AFM, KPFM, UHV, Graphene, Silicene, 2D material, MBE growth.

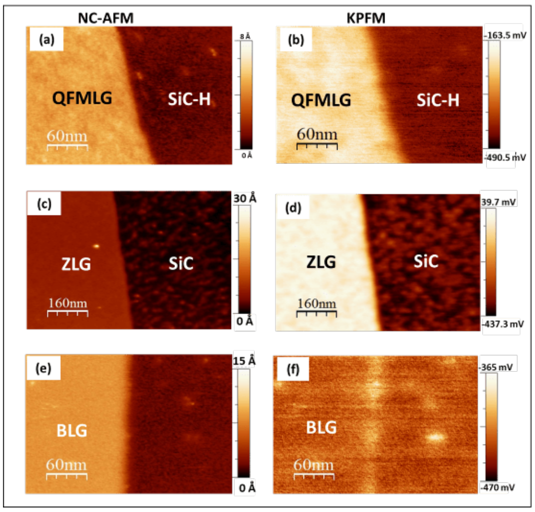

Figure 1: Nc-afm ((a),(c),(e)) and KPFM (((b),(d),(f) images of different structure of graphene on 6H-SiC(0001).

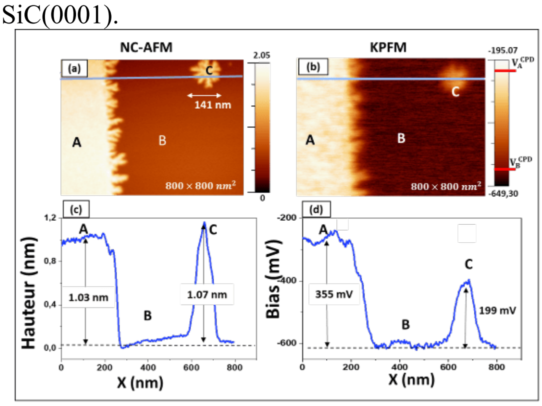

Figure 2: Nc-afm (a) and KPFM (b) images of silicon growth on Graphene/6H SiC(0001).(c) topographic and (d) potential line profil.

References:

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Optimization of the terminations and stability of polyynes through ns-pulsed laser ablation in organic solvents

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Abstract:
Beyond the most known allotropes of carbon, polyynes represent sp-hybridized carbon systems, linear chains made by alternating single and triple bonds. They recently attracted a large interest because of their predicted remarkable mechanical and electronic properties [1]. In this scenario, pulsed laser ablation in liquid (PLAL) appeared to be the best one-step physical synthesis method, able to produce long chains and to tune their terminating groups.

In this framework, we investigated ns-PLAL testing different organic solvents with the goal of providing different termination to carbon-chains. Preliminary UV-Visible absorption spectra revealed the presence of polyynes. The mixtures were further analyzed by high-performance liquid chromatography (HPLC) that unveiled the existence of long H-terminated polyynes, up to $HC_{22}H$. Different terminations were also recognized, such as methyl- and cyano-capping, until $HC_{18}CH_3$ and $HC_{12}CN$ respectively. Through HPLC, we were able to collect size- and capped-selected polyyne solutions for further analysis.

The capping-assignation of size-selected polyynes was also tested by means of surface-enhanced Raman spectroscopy (SERS), exploiting silver nanoparticles colloids. We identified the characteristic ECC peak of polyynes, due to C-C stretching of the *sp*-chain, in the range 1900-2200 cm^{-1} (Fig. 1) , as predicted by DFT simulations. Moreover, we were able to distinguish between different terminating group, looking at the shape and position of the ECC band.

We accomplished the synthesis of long-polyynes by means of PLAL in organic solvents. We are planning *in-situ* SERS measurement that will grant a better insight in the functionalization of polyynes termination groups and in the ablation process. These progresses are necessary for future optical and electronic applications of polyynes.

Keywords: carbyne, polyyne, sp-carbon, pulsed laser ablation, cyano-polyyne, methyl-polyyne, Raman spectroscopy, surface.enhanced Raman spectroscopy.

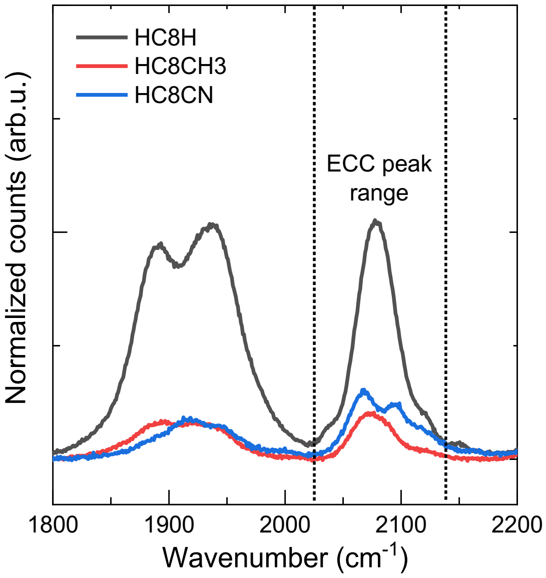

Figure 1: SERS spectra of differently-capped polyynes of equal *sp*-chain length. The region of the ECC peak is enclosed between two dashed lines. The effects of the different terminations were to change both the position and the shape of the peak, introducing a significant asymmetry in the cases of both methyl- and cyano-polyynes.

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Electorospun nanofibers with photocatalytic particles for carbon sorption

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Abstract:
Current global climate challenge is directly connected to carbon dioxide emmisions to the atmosphere. Using fossil fuels as a conventional and efficient source of energy we daily increase the CO_2-footprint. One of the most promising approaches to reduce carbon dioxide concentration in the atmosphere are membranes for carbon capture and, ideally, utilization (CCU).[1] Nanostructured materials that have a high surface-to-volume ratio demonstrate unique chemical, physical and mechanical properties that are on demand in energy and environmental applications.[2] One approach to produce nanofibers is electrospinning. In particular, needleless electrospinning has a potential for the production of nanofibers at high-throughput that is essential for such industrial applications.[3] In this work we used needleless electrospinning from the blade to produce nanofibers for carbon capture and utilization applications. We have optimized the high-throughput electrospinning process for various industrial grade polymers such as polyvinyl alcohol (PVA), polyacrylonitrile (PAN) and blends of PAN with polyethylene oxide (PEO) and polyethyleneimine (PEI) achieving the nanofiber production rates of up to 12 g/hr. Moreover, needleless electrospinning allowed us to produce hybrid nanofibers loaded with photocatalytic titanium dioxide (TiO_2) nanoparticles with very high loading capacity up to 50 % of the mass of polymer (Figure 1). Such hybrid nanofibers with photocatalytic properties have tremendous applications not only in the carbon utilization but also in various other environmental applications.

Keywords: electrospinning, needleless electrospinning, membrane, nanofibers, carbon sorption, capture, photocatalytic conversion, environmental applications.

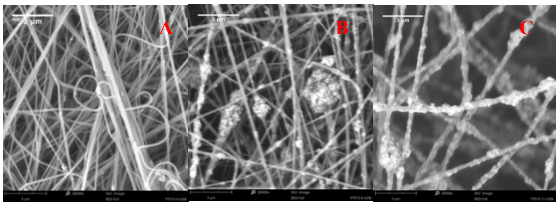

Figure 1: SEM image of PAN/PEO fiber incorporated with titanium dioxide nanoparticles: (A) 3 % loading, (B) 30 % loading, (C) 50 % loading

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Silica and alumina-silica based aerogels reinforced with aramid fibres as promising candidates for Space applications

7

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Abstract:

The development of effective external thermal insulation (ETI) systems of cryogenic storage tanks for launch rockets, used in the aerospace industry, is still a challenge, due to the imposed extreme conditions in Space environment. For these applications, a material with reduced weight that combines both good thermal insulating and mechanical properties is required. In this sense, silica-based aerogels emerge as excellent candidates, since they display low density (<150 kg m^{-3}), very low thermal conductivities (0.015 – 0.025 W m^{-1} K^{-1}) and non-flammable character [1,2]. However, this type of material is inherently brittle and presents poor dimensional stability for temperatures above 600 ºC, which may limit its application.

The AeroXTreme project is developing some strategies, namely reinforcement by organic thermally stable fibers (aramid) [3] and introduction of a higher dimensional thermal stability refractory phase (alumina) [4], which are adequate alternatives to overcome the mentioned issues.

Systems containing aramid fibres (pulp, longer fibres and felt) as reinforcement in silica aerogels synthesized from a TEOS-VTMS precursors [3, 5] were previously optimised. The aerogels containing these fibres had low bulk density values, down to 150 kg m^{-3}, and reached thermal conductivities bellow 30 mW m^{-1} K^{-1}; they were also thermally stable up to 550 °C. It was observed that *para*-type short length and *meta*-type elongated fibres produce stiffer composites with best insulation performance. The compliance and suitability of these aerogels for Space use was confirmed after submission to Standard tests for Space materials qualification (thermal cycling and outgassing).

To overcome the densification of silica aerogels at higher temperature and improve their performance for application in these environments, an alumina phase was introduced in the nanocomposites in small amounts by using aluminum chloride and tri-sec-butoxide as alumina precursors. The influence of the Al/(Si+Al) ratio, up to 15 mol%, was investigated in terms of structural-morphological and thermo-mechanical properties. The aerogels with aluminum chloride had lower densities (~130 kg m^{-3}) and thermal conductivities (~30 mW m^{-1} K^{-1}), much more promising when compared with tri-sec-butoxide based ones. They could also suppress the weight loss above 500 ºC due to silica defects elimination, as aimed.

Keywords: aerogel composites, alumina-silica, thermal insulation, Space

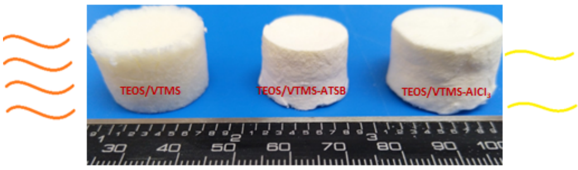

Figure 1: Picture of different silica and alumina-silica aerogel composites.

Acknowledgements:

Work developed under the project AeroXTreme (CENTRO-01-0145-FEDER-029533) - High-performance silica aerogel nanocomposites for insulation under extreme temperature Space environments, co-funded by Foundation for Science and Technology (Portugal) and the European Regional Development Fund (ERDF), through the Regional Operational Program of the Center of Portugal (Centro2020).

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Biotech France Session I. C

Synthetic Biology for a Sustainable World

Richard I Kitney

Imperial College London, UK

Abstract:
To address climate change, the world's economies need to progressively move from a non-sustainable to a sustainable industrial model. The current model comprises oil-based feedstocks as its input, feeding through synthetic chemistry to industrial processes and products. The sustainable model uses bio-based feedstocks feeding through synthetic biology to industrial processes and products. Key elements of how synthetic biology differs from traditional biotechnology will be addressed and some industrial examples given. Biofoundries and their development - in terms of high levels automation, the application of AI and machine learning - will be described. Biofoundries need to be part of the process of optimisation of gene circuits. Examples will be given of how optimisation techniques are being applied to bio design. An example of optimisation will be discussed in relation to lycopene and vaccine development. Strategy for distributed design and manufacturing will also be outlined.

Microbial Electrochemical Technologies Enable New Biotechnological Processes

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[1] Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany

Abstract:
More and more microbes are discovered that are capable of extracellular electron transfer, a process in which they use external electrodes as electron donors or acceptors for metabolic reactions (Figure 1). This feature can be used to overcome cellular redox limitations and thus optimizing microbial production. The technologies, termed microbial electrosynthesis and electro-fermentation, have the potential to open novel bio-electro production platforms from sustainable energy and carbon sources. However, the performance of reported systems is currently limited by low electron transport rates between microbes and electrodes and our limited ability for targeted engineering of these systems due to remaining knowledge gaps about the underlying fundamental processes. Metabolic engineering offers many opportunities to optimize these processes [1].
Over the last decade, we have explored the use of microbial electrochemical technologies to drive processes in *Clostridium autoethanogenum* [2], *Pseudomonas putida* [3], and lately also *Synechocystis* PCC 6803 [4]. This included cathodic processes (electron delivering) and anodic processes (electron accepting). The different strains show distinct phenotypes under the respective regime allowing the shift of central metabolism based on the redox potential at which electrons are offered or withdrawn, respectively. This shows that metabolic fluxes could be redirected based on voltages applied to the system. We believe that this promises to become a great new tool in the toolbox for metabolic engineering and steering of pathways for biotechnological applications.

Keywords: Microbial Electrochemical technologies, Electrofermentation, Biophotovoltaics

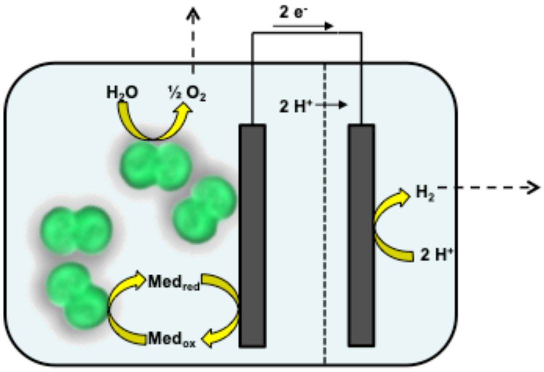

Figure 1: Bacteria interacting with electrodes in MET systems turning substrates into products while balancing t metabolism via electrodes (here a phototrophic cyanobacterium)

References:

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The potential of microbial biotechnology toward a low-carbon bioeconomy

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[1] Aston University, Energy and Bioproducts Research Institute, Birmingham, UK
[2] Aston University, Aston Institute of Materials Research, Birmingham, UK

Abstract:

Biotechnology is transforming traditional industry through the use of living organisms, such as microbes or enzymes, to produce biotechnological products and materials in a cleaner, safer and more sustainable way. We can take advantage of the benefits that biotechnology offers to face new challenges such as climate change, sustainable production of raw materials and clean energy or the availability of new health solutions to increase people's quality of life. Biotechnology is reshaping the future by creating new and innovative products and providing more efficient and sustainable processes in sectors such as food, chemical, cosmetic, pharmaceutical, plastics and energy, and is also offering innovative solutions for waste treatment and pollution reduction. With a 20% annual growth, biotechnology is expected to be a mainstream technology in the bioenergy and bio-based products sectors.

Here, we will introduce how researchers at the Energy and Bioproducts Research Institute and Supergen Bioenergy at Aston University address key research challenges to develop sustainable bioenergy systems and bio-based products through an interdisciplinary and systems approach (Figure 1) and, discuss the challenges and opportunities for microbial biotechnology in the low-carbon bioeconomy context. We will showcase some of our ongoing research projects on the exploitation of microbial factories for the production of biotechnological products such as enzymes for biodiesel production, biopolymers for packaging and magnetic nanoparticles for energy and healthcare applications.

Keywords: bioenergy, climate change, industrial biotechnology, bio-based products, low-carbon, bioeconomy, biodiesel, bioplastics, magnetosomes.

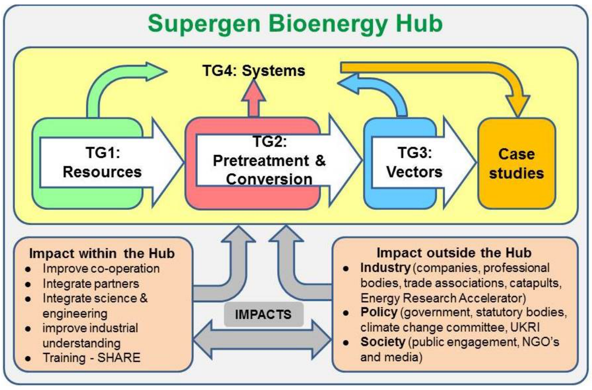

Figure 1: Figure illustrating how The Supergen Bioenergy Hub works with academia, industry, government and societal stakeholders to develop sustainable bioenergy systems that support the UK's transition to an affordable, resilient, low-carbon energy future.

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Scaling up from lab to industrial scale minimizing performance loss: From simulation to strain engineering of *E. coli*

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Abstract:

Successful metabolic engineering aims to create microbial hosts that produce the targeted compound under industrial production conditions. Often enough, large scale bioreactors suffer from non sufficient mixing creating micro-environmental heterogeneities. Fluctuating cells experience the resulting gradients (e.g. of substrates) as repeated stimulations, triggering metabolic and transcriptional responses. As a consequence, the key performance criteria TRY (titer, rates, yields) may deteriorate.

In order to predict the large-scale performance of novel producers proper scale-down tests should be performed providing data for strain characterization. Subsequently, data driven multi-scale simulations should be applied unravelling the cellular response. Thereof, biochemical engineering measures could be deduced for optimizing bioprocesses and bioreactor design. Alternately, metabolic engineering targets could be formulated to improve microbial robustness.

Scale-down experiments: A series of scale-down experiments mimicking large scale conditions was performed with *E. coli* (Loeffler, Simen et al., 2016). Thereof, metabolic and transcriptional dynamics were identified allowing the conclusion that the repeated on/off switching of stringent response caused additional ATP needs.

Large-scale simulation: *E. coli*'s performance was simulated for an industrial bioreactor. Based on comprehensive data sets, the transcriptional regulation predicted the delay between fast metabolic response versus transcriptional readout. Accordingly, stress patterns of *E. coli* transcriptional response occur in well mixed bioreactor zones which may have not been expected without applying the multiscale simulation approach. Simulations mimic the population heterogeneity often observed in industrial-scale settings.

Strain engineering for large scale application: Based on the experimental findings *E. coli* SR, a stringent response knockdown strain, was engineered. Exposure to said large-scale conditions revealed a strongly reduced transcriptional response compared to the wildtype (Ziegler et al., 2020). Besides, further exploitation of the transcriptional dynamics (Loeffler et al. 2016) lead to the genome-reduced strain *E. coli* RM214. Taking the plasmid encoded eGFP production as a proxy for metabolic production capacities, *E. coli* RM214 revealed superiority by showing 45% higher eGFP production rates than *E. coli* wildtype when being exposed to large-scale conditions (Ziegler et al., under review).

Keywords: scale up, computational fluid dynamics, stringent response, *E. coli*.

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Model-informed biopharmaceutical glycoengineering

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Abstract:

Asparagine (N)- linked glycosylation is a key determinant of the safety and efficacy of many blockbuster monoclonal antibody (mAb) biopharmaceuticals. Specifically, the presence of β4-linked galactose residues on the N - glycans of mAbs is known to increase their oncolytic activity but, simultaneously, is also known to vary substantially across commercial manufacturing lots, leading to quality assurance concerns for these products. mAb β 4-galactosylation variability arises from two bottlenecks: (i) limited availability of UDP- Gal, the metabolic co-substrate required for product β4- galactosylation and (ii) limited availability of β4GalT, the Golgi-localised enzyme which catalyses product β4-galactosylation. Due to the multiplicity of factors governing β4-galactosylation, robust strategies addressing both metabolic and cellular machinery bottlenecks are required to ensure the glycosylation-associated quality of mAbs. This presentation will outline my team's recent work on deploying computational modelling tools to rationally engineer and control biopharmaceutical glycosylation quality.

The potential of hybrid process modeling and digital twins to master the goals of industry 4.0 in bioprocessing

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Abstract:

Hybrid modeling is emerging as a pragmatic solution that combines the advantages of the two modeling paradigms, and have been promoted as a PAT to realize QbD. The concept has been extensively investigated for microbial cultures over three decades. Few hybrid models have also been developed for mammalian cell cultures, though initially in more explorative academic setting.
In this contribution, we show how hybrid modeling approaches can be exploited to efficiently model, improve understanding and optimize upstream and downstream mammalian bioprocesses. Industrial case studies will thereby present the potential of this technology to accelerate and robustify process development. Moreover, industrial examples will illustrate the additional advantage of hybrid models embedded into digital process twins for integrated, in silico process design and scenario analysis as well as optimal operation and cross-unit prediction.

Keywords: hybrid modeling, bioharma, cell culture, chromatography, digital twin, machine learning.

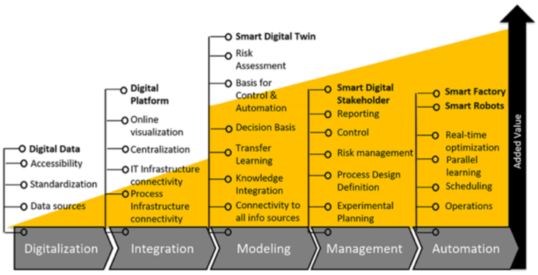

Figure 1: Added value and solution concepts achievable at different levels of digital transformation in the biopharmaceutical process industry.

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Gasification of biomass: Characterisation of spelt husk briquette and pellet

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Abstract:
Biomass from horticultural residues are getting increased consideration as feedstocks for renewable energy. Spelt wheat is an ancient crop which is experiencing a restored enthusiasm for its apparent medical advantages when compared to other common grown crops. Spelt husks were categorized for their potential as a renewable energy feedstock and the effects of compacting temperature (i.e. 20, 50, 80°C), pressure (i.e. 150, 200, 250MPa) and particle size (<1.00, <2.36mm and mixed particles (MR)), on briquette and pellet properties were studied.

It was found that an increase in compacting temperature and pressure resulted in increased density, impact resistance and compressive strength of both pellets and briquettes. However, the highest density was achieved for pellets using <1.00mm particle size and for briquettes <2.36mm particles sizes. For briquettes density, impact resistance, and compressive strength were significantly increased with increasing compacting temperature (20–80°C) and compacting pressure (150–250 MPa). Density of briquettes increased from 890.94 to 1223.34 kgm^{-3} with an increase in the tested compacting temperature (20–80°C) and particle size (<1.00 to MR). There was no any admixture or additives utilized in the process. Spelt husks contained 10.58% moisture, 6.32% ash, 73.29% volatile matter, 9.81 % fixed carbon with an energy content of 17.56 MJkg^{-1}. From chemical analysis, it was found that the spelt husks have 45.30 % carbon, 5.95% hydrogen, 1.81 % nitrogen and 45.95% oxygen. Furthermore, the pyrolysis temperatures had influence on the gasification step which enhanced the syngas composition thereby increasing the hydrogen content in the gasification step. Hydrogen content increased as the pyrolysis temperature increases whilst the methane content was decreasing at the gasification step i.e. H_2 content increased from 33.3 to 35.0 mol% (raw spelt husks), 25.6 to 31.3 mol % (spelt husks pellets) and 35.5 to 38.4 mol% (spelt husks briquettes) respectively. This study further suggested that the use of pre-treated spelt husks (spelt husks briquettes) was more preferred for gasification because it yielded the highest HHV of 27.9 MJkg^{-1}, highest gas yield of 76.6 wt% and highest H_2 content of 38.4 mol% at the gasification step.

Keywords: Spelt husks, density, impact resistance, compressive strength, particle size, compacting temperature, pressure, hydrogen content, methane, gasification.

Acknowledgement: This work is supported by Petroleum Technology Development Fund (PTDF) Nigeria.

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Removal of Poisonous Arsenic (As) from Drinking Water in Developing Countries by using *Wasted Coffee Beans*

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Abstract:

There are so many people suffering from ***drinking water problems*** in the World. For example, in Bangladesh **(see Fig.1)**, more than half the nations (>70,000,000) are taking drinking water from the underground. A trace amount of **As (arsenic)** (poisonous) is contained in this water. By taking it continuously, serious diseases have developed after for a long time (~30years). Patients suffering from not only surface cancer but also inner organs one have been reported. The problem is that the diseases are occurring in the very poor people, the bottom class. They can't buy purification apparatus or system. It takes a lot of money to buy it. It has been strongly required that someone will save their lives.

Coffee beans are very effective material for this purpose. It showed powerful adsorbent property for the selective removal of As (arsenic) from among underground drinking water **(Fig.2) [1].** Not only fresh beans but also wasted ones showed excellent property. Of course, other agricultural materials such as rice shed, wheat one, and dried grass, showed good results after some carbonization treatment (>300°C) **[2]**, but coffee beans are outstandingly good. No additional treatment or handing is necessary. Here we present the experimental data and hope to spread this information to the World.

Keywords: Water purification, underground-dinking water, contamination, poisonous As, wasted coffee beans, selective removal, adsorption.

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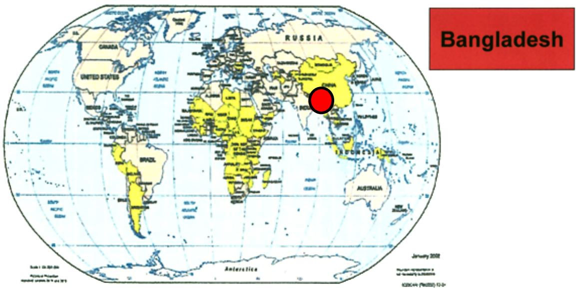

Figure 1. World map indicating the location of As water problems (yellow colored countries). Red circle does Bangladesh (*old* East-Pakistan).

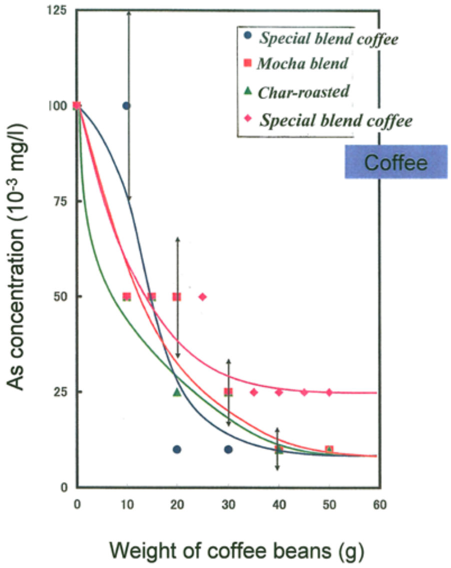

Figure 2. Adsorption behavior of coffee beans. More than 80-90% of As in the underground water was removed only by passing through coffee layer packed in the glass reactor vessel. Blue cicle (*special blend*) is the results of recycled coffee.

Nanotech / NanoMetrolgy Joint Session II. A: Workshop on VIMMP project - Virtual Materials Marketplace (H2020 GA 760907)

Knowledge representation for materials modelling marketplaces

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Abstract:

By introducing a common representational system for data and metadata pertaining to a domain of knowledge, multiple data sources and platforms, *e.g.*, workflow management systems, become interoperable at the semantic level [1]. The present work applies this approach to the field of materials modelling and adjacent domains of knowledge. The Virtual Materials Marketplace (VIMMP) project, in which a digital marketplace for services in materials modelling is constructed and launched, employs a system of marketplace-level domain ontologies to characterize services, models, and material properties, *cf.* Fig 1. This work presents the ontologies from VIMMP and illustrates their use in practice, focusing both on data ingest and retrieval at the digital marketplace infrastructure itself and on their potential contribution to platform interoperability [2]. Additionally, it is argued that open platforms require pragmatic interoperability, *i.e.*, community-governed agreements on good practice that estab-lish minimum standards and shared evaluation criteria for processes and roles. For this purpose, if ontology-based semantic interoperability is al-ready present, the same ontologies can be used. This is illustrated here by the role of the transla-tor (*i.e.*, facilitator) in computational molecular engineering and procedural definitions for the process of translation, which refers to mapping industrial research and development problems onto solutions by modelling and simulation [3].

Acknowledgment. The VIMMP (Virtual Materi-als Marketplace) project is funded from the Eu-ropean Union's Horizon 2020 research and inno-vation programme under grant agreement no. 760907. This work was facilitated by the activi-ties of the Innovation Centre for Process Data Technology (Inprodat e.V.), Kaiserslautern.

Keywords: Molecular modelling and simulation, ontology engineering, semantic technology, digitalization, materials modelling, computational molecular engineering, process data technology.

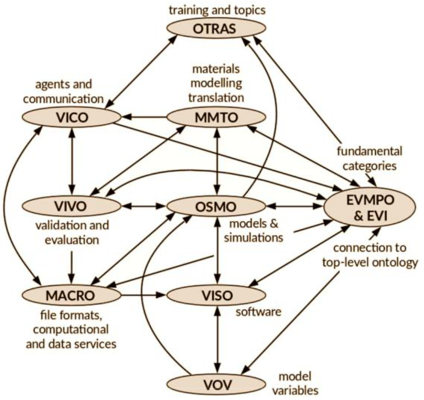

Figure 1: System of marketplace-level domain ontologies developed in VIMMP [2].

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Numerical simulation of food emulsion production: the mayonnaise case

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Abstract:

Mayonnaise is a stable food emulsion with a high content of the disperse oil phase. The production of mayonnaise is a typical mixing process, in which the ingredients (i.e. egg yolk, vinegar, oil and water) are first mixed in large stirred vessels at moderate rotational speed. Then the formed emulsion is finally fluxed into a high-shear mixer, where the droplets undergo breakage until the final size distribution is reached; this last step is crucial to fine tune the droplet size distribution, in order to have a final product with the desired features. Therefore the prediction of the final droplet size distribution is essential for the determination of the properties of the final product, such as structure, stability over time, taste and color.

In this work, we aim to simulate the last step of the production process by means of a multiscale model composed by (a) a Computational Fluid Dynamics approach coupled with a Population Balance Model (CFD-PBM) [1], to properly describe both the non-Newtonian dynamics of the emulsion and the evolution of the droplet size distribution (b) a Dissipative Particle Dynamics (DPD) or Molecular Dynamics (MD) approach to describe the interfacial properties of the emulsion. A schematic representation of the macroscale investigated apparatus, so called cone mill mixer, is reported in Figure 1. It is constituted of a solid conical frustum rotor inside a slightly larger stator of the same shape, forming a small gap in which the emulsion flows and experiences high-shear rates, due to the high rotational speed of the rotor. For this particular system experimental data are available in the literature [2].

This particular workflow will be useful to develop an open simulation platform for generic multiscale and multiphysics simulations, where the computational codes aiming at different parts of the physics are linked and coupled.

Keywords: food emulsion, droplet coalescence, droplet breakup, CFD simulation, population balance modeling.

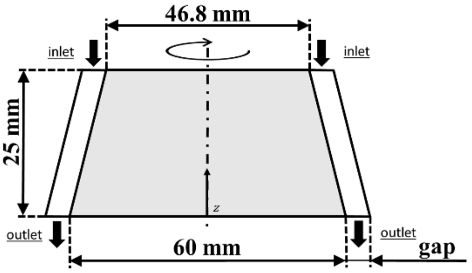

Figure 1: Sketch of the investigated cone mill mixer.

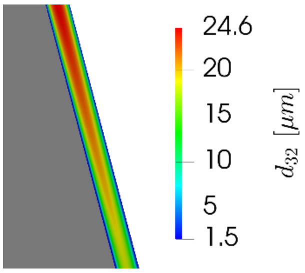

Figure 2: Trend of the mean oil droplet diameter along the section of the cone mill mixer.

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Acknowledgment

This work has been developed in the context of the Virtual Material Marketplace project (www.vimmp.eu). The project leading to this application has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 760907.

Dispersive mixing of filler agglomerates in a polymer compounding operation: A CFD-DEM investigation

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[2] Continental Reifen Deutschland GmbH, Hannover, Germany

Abstract:

The compounding of polymeric materials frequently requires the incorporation of solid filler particles in order to enhance the mechanical properties of the final product. Most of the fillers exist in the form of large agglomerates which, during the mixing process, are broken down into smaller fragments and uniformly distributed into the matrix. [1]

Previous research has generally focused on the investigation of the flow field in the mixing equipment and only few attempts have been made in the analysis of the breakup behavior of the agglomerates, with most of them adopting severe simplifications either on the flow field or on the agglomerate morphology.

In this work we present a numerical approach able to investigate accurately the dynamics of the process. The method is based on a combination of Computational Fluid Dynamics (CFD) and Discrete Element Method (DEM) simulations. CFD simulations are carried out to compute the flow field inside a typical internal mixer; at this stage, the agglomerates are treated as tracer particles and their trajectories are computed and feeded to a DEM code, together with the viscous stress components experienced during the motion. The DEM model, built in the framework of Stokesian Dynamics, takes into full account the disordered structure of the agglomerates and returns the normal force acting on each single monomer-monomer contact. From this information the occurrence of breakup can be readily determined, by comparing the tensile force with the critical pull-off force required to break the contact.

Simulations returned profound insight into both the breakup kinetics and the morphology and size distribution of the broken agglomerates, which may be used for the design and choice of operative conditions in polymer compounding processes.

Keywords: polymer compound, Banbury mixer, CFD simulation, Stokesian Dynamics, agglomerate breakup, dispersive mixing.

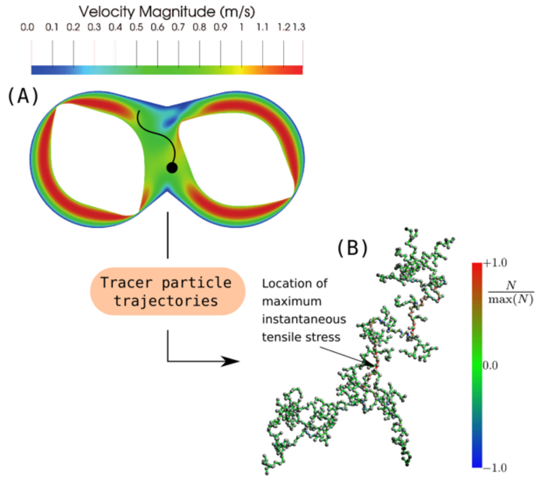

Figure 1: Figure illustrating the adopted modelling approach. (A) Velocity magnitude contour plot from CFD simulation performed by using Ansys Fluent 19.2 The trajectory of a set of tracer particles is obtained by interpolating the computed flow field. (B) DEM simulations are used to evaluate the tensile internal stress acting at inter-monomer contacts along trajectories.

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Acknowledgment

This work has been developed in the context of the Virtual Material Marketplace project (www.vimmp.eu). The project leading to this application has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 760907.

Salt-induced self-assembly of fibrinogen nanofibers: How the development of new biomaterials can benefit from a virtual materials marketplace

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Abstract:

Fibrinogen is a blood plasma protein that is essential in blood clot formation and tissue repair. By thrombin-mediated cleavage fibrinogen is converted into fibrin, which polymerizes into a fibrous network that avoids excessive bleeding and promotes wound healing. Although such fibrin networks can been assembled under *in vitro* conditions they require the use of expensive thrombin and often suffer from fast degradation when used as scaffold materials.

Recently, we were able to prepare fibrous fibrinogen structures without using thrombin by introducing salt to fibrinogen solutions followed by a controlled drying step.[1,2] During this novel process of salt-induced self-assembly fibrinogen nanofibers could be assembled on different surfaces. Via tailored crosslinking we were also able to prepare free-standing fibrinogen nanofibers, which demonstrates the versatility and high potential of these new biomimetic scaffolds for future wound healing applications.

So far, little is known about the underlying mechanisms of fibrinogen fiber formation during self-assembly. Therefore, we performed secondary structure analysis of fibrinogen scaffolds using Fourier transform infrared (FTIR) and Circular dichroism (CD spectroscopy). This analysis revealed a partial transition from α-helical structures to β-strands upon fiber formation. Moreover, when no salt was present a planar film of fibrinogen was observed in comparison to nanofibers, which assembled when salt was added (Figure 1). During optimization of the self-assembly conditions, we also found an influence of protein concentration and pH on the secondary structure of self-assembled fibrinogen nanofibers. Interestingly, a staining of nanofibrous fibrinogen with thioflavin-T revealed no amyloid formation, which is an important prerequisite for the development of non-pathogenic fibrinogen scaffolds for tissue engineering. Although we could already identify an influence of salt addition on the morphology and secondary structure of self-assembeld fibrinogen scaffolds, it is still not understood in detail what is the major driving force underlying fiber formation. [3]

To complement our experimental findings and to test our hypothesis that the presence of salt plays a major role during fibrinogen fiber formation *in vitro* we also used the materials modeling platform VIMMP to find similar case studies. Using the translator tool[4] of this digital, interactive platform we identified new possible collaborations for modeling the salt-induced self-assembly process across different length scales. Based on these simulations it is our aim to gain fundamental insight into the underlying principles of fibrinogen fiber formation *in vitro*. Understanding the multiscale mechanisms during fibrinogen fiber assembly *in vitro* will enable us to tailor multifunctional fibrinogen scaffolds for versatile applications in tissue engineering in the future.

Keywords: fibrinogen nanofibers, circular dichroism spectroscopy, infrared spectroscopy, salt-induced self-assembly, conformational changes, translation router, modeling solutions.

Acknowledgement: We gratefully acknowledge funding via the Emmy Noether Program of the German Research Council (grant no BR5043/1-1) and via the program Fraunhofer TALENTA start.

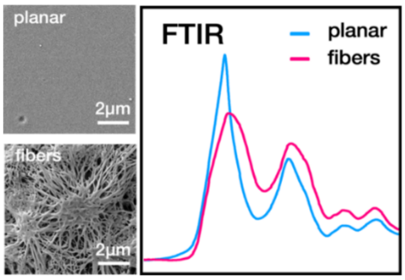

Figure 1: Correlation between the morphology of self-assembled fibrinogen scaffolds and the secondary structure accessed by SEM and FTIR.

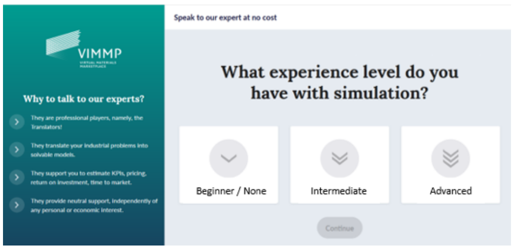

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Figure 2: VIMMP translation router app to facilitate the translation of key research questions into a solution via materials modeling

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Mesoscopic Modelling of Interactions of Structured Fluids with Soft Surfaces

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Abstract:

Numerous liquid products in sectors of personal care or household cleaning are colloidal systems characterised by rich phase diagrams. These liquids are 'structured' to produce thickened, metastable suspensions whose rheology is sensitive to many aspects such as its composition or the solution temperature. Among the rheologies, surfactant lamellar phases and their interactions with soft surfaces play an important role in industrial and household products such as fabric softeners or hair conditioners. Understanding surface adsorption of surfactant lamellar phases under various conditions as well as the effect of the composition of the lamellae is therefore of utmost importance, because it seriously affects the product's efficacy. Using the computer simulation method known as the Dissipative Particle Dynamics with a recently developed generic forcefield[1], we have performed a preliminary but extensive parametric study of adsorption of surfactant lamellae on a polymer brush that mimics the surface of a human hair. This study is important to discover trends in composition and conditions that lead to ideal consistency of the liquid and subsequently enhanced performance of the final product. The surfactant lamellae comprise of a mixture of fatty alcohol (cetyl, stearyl, or dodecyl alcohol) and ionic surfactant (cetrimonium chloride or dihexadecyldimethylammonium bromide) in various concentrations, whereas the polymer brush comprises of methyleicosanoic acid that is found on the surface of human hair[2]. We set up the brush density to correspond to that on the surface of the human hair; however, to explore general trends we also performed simulations with higher and lower brush densities. We also varied the solution temperature to observe the transition between gel-like and liquid lamellar phases. By careful analysis, we have identified a range of conditions and system compositions for further study.

VIMMP project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 760907.

Keywords: polymer brush, surfactant, structured fluids, dissipative particle dynamics

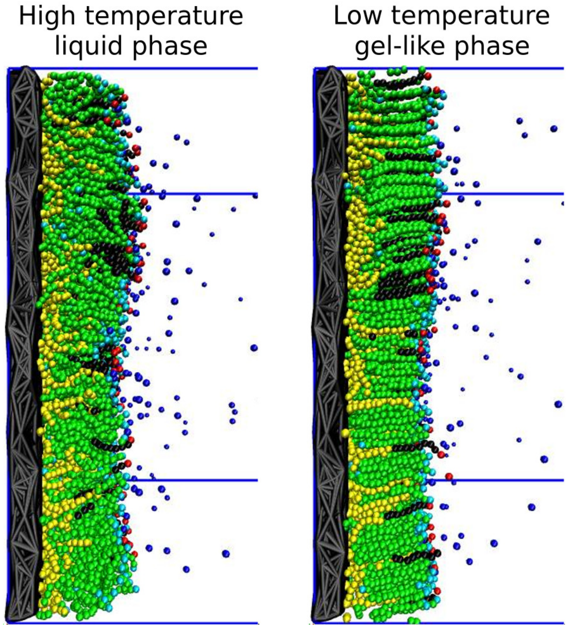

Figure 1: Temperature dependent structural differences.

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Calculation of the work of adhesion of polyisoprene on graphite by molecular dynamics simulations

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Abstract:

Elastomeric compounds are reinforced with fillers such as carbon-black and silica to improve mechanical, dynamical and tribological properties. The stability and physical properties of these materials are dominated by the intermolecular interactions occurring at the polymer/particles interface that determine the magnitude of the polymer/particles adhesion.

In this talk we present the evaluation of the solid-liquid interface tension and of the work of adhesion using molecular dynamics simulations for a system composed of graphite/Polyisoprene 100% cis-1,4 within a range of molar masses and temperatures. We employ a simulation strategy for estimating the surface tension of fluid/vacuum and fluid/solid interfaces that uses directly the local stress fields in the Irving-Kirkwood formalism. Using such procedure, we decompose the stress field into the individual components of the stress tensor and correlate them with the values of the work of adhesion in the different systems analysed.

Acknowledgment

The VIMMP (Virtual Materials Marketplace) project is funded from the European Union's Horizon 2020 research and innovation programme under grant agreement no. 760907.

Keywords: Work of adhesion, polyisoprene, Carbon black, Stress Profile, graphite.

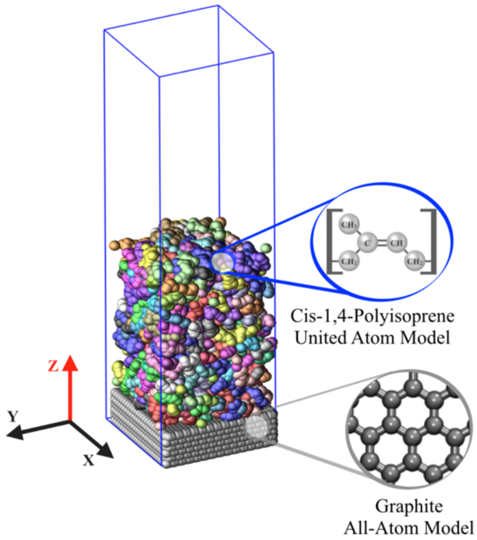

Figure 1: Molecular Dynamics snapshot of one of simulated systems, *i.e.*, thin polyisoprene melt film on contact with graphite.

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Nanotech France Focused Session on Nanocoatings / Thin films and Nanostructured Surfaces

Synthesis of Nanostructured Metallic Foams by Plasma Electrolysis Deposition

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Abstract:

Within the framework of fundamental physics studies at CEA, laser target experiments are conducted to investigate laser-matter interactions. Some of these experiments require metallic foams samples in a milimetric scale with an apparent volumetric mass within few hundreds milligrams per cube centimeters. Metallic foams materials are developed and studied since few years for their unique properties offered by their aerated structure. For example, due to a high specific surface, metallic foams could find applications in batteries, supercapacitors, as well as chemical sensors. However, all the metallic foams obtained by the processes referenced in the literature do not meet the specifications needed for laser experiments. This is why, the CEA has developed a new and innovative technique to synthetize metallic foams by plasma electrolysis deposition [1]. This process consists in applying a voltage within the 20-100V range at a cathode immerged in a solution containing metallic ions. Under these specific conditions, a uniform gaseous sheath is created around the cathode which is then isolated from the liquid. Due to the high electrical field applied at the electrode surface, several electrical plasma discharges are formed between the cathode and the gas/liquid interface. When the electrical discharges meet the solution, metallic cations are reduced to form metallic strands about 100 nm in diameter. The formed strands are all interconnected together to form metallic foam with micrometric porosities [2]. A few millimeters wide foam with a volumetric mass up to 100mg/cc is obtained in about 10 seconds which is very fast compared to classical electrochemical deposition techniques. The foams synthetized can be made up of pure metals (Cu, Au, Pt …) or alloys (AuCu …) in accordance to the metallic ions diluted in the solution. Our work aims to understand the physico-chemical mechanisms involved in the foam growth and leading to the cristallisation of the strands. We report the presence of plasma streamers and their influence on the foam strands shape.

Keywords: Metallic Foam, low density nanomaterial, plasma electrolysis, plasma streamers

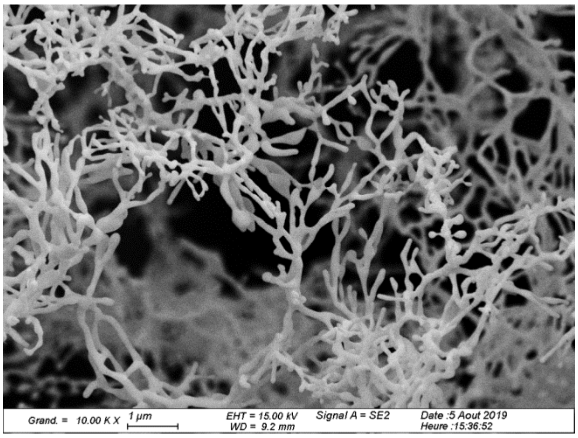

Figure 1: SEM Picture of gold foam (80mg/cc) obtained by plasma electrolysis deposition. We see fully cristallised strands about 100nm in diameter with their characteristic shape resulting from the plasma streamer propagation in the electrolyte.

References:

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One-step Templateless Electrosynthesis of Nanostructured PEDOT films

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Abstract:

Conducting polymers such as poly(3,4-ethylenedioxythiophene) (PEDOT) and polypyrrole (PPy) have been widely used as electrode materials for supercapacitors. PEDOT is a promising electrode material because of its high electrical conductivity, great environmental stability and high cycling stability. Nanostructuration of the polymers can provide better performances of volumetric swelling and shrinking during charge/discharge processes. We have already described the templatefree electrosynthesis of PPy nanostructures [1, 2] but to the best of our knowledge, the easy templateless electrosynthesis of nanostructured PEDOT in aqueous solutions has not been reported yet. This work demonstrates a simple one-step templatefree electrosynthesis method of preparing various structured PEDOT films which show good specific capacitance and cycling stability. By varying some experimental parameters, we have obtained various nanostructures: nanofiber networks, nanorods, nanospheres and nanowires of PEDOT (Figure 1). These structures were obtained by simply adjusting the applied potential and the composition of the monomer solution i.e. the concentration of weak-acid anions such as HPO_4^{2-} and the concentration of non-acid anions such as ClO_4^-. The growth mechanism of the nanostructured PEDOT films will be discussed. At the very beginning of the process, water oxidation takes place which leads to the formation of hydroxyl radicals and to the evolution of O_2. Moreover, the nanostructured PEDOT films show high specific capacitance (~100-200 F/g) and cycling stability (capacitance retention is about 90% after 1000 scans) (Figure 2). Therefore, the nanostructured electrogenerated PEDOT films could be used for many applications, such as supercapacitors.

Keywords: PEDOT, nanostructured conductive polymers, electrosynthesis, supercapacitance, cycling stability.

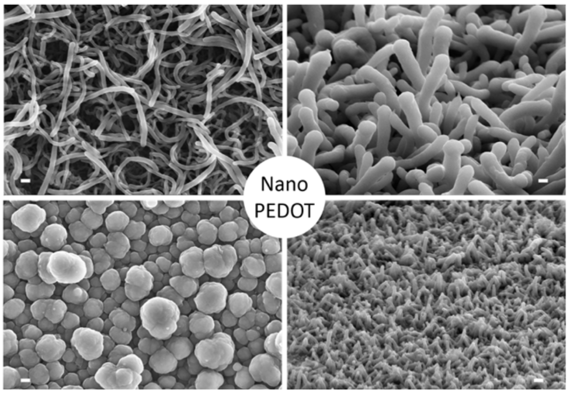

Figure 1: SEM micrographs of various morphologies of PEDOT obtained using a templateless electrochemical route. Scale bar : 200 nm.

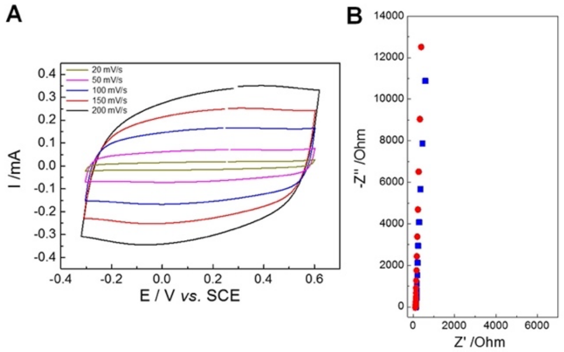

Figure 2: (A) I-E curve of a nanostructured PEDOT film at various scan rates, in $LiClO_4$ 0.1 M. (B) EIS of a nanostructured PEDOT film. Blue squares just after film synthesis ; red circles after 1000 scans at 20 mV/s in $LiClO_4$ 0.1 M.

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Influence of element composition on thermal stability and oxidation resistance of Ti-Cr-Mo-Ni-N coatings

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Abstract:

Nowadays actively studied multicomponent coatings based on nitrides of transition metals. This interest is associated with the high and unique properties of coatings that can be obtained. Of particular interest are the (Me, Me) N-Ni / Cu systems, where, as a result of the complete solubility of the components in each other, nitride grains of alternating compositions are formed in the nickel matrix. In this work, the thermal stability and heat resistance of the Ti-Cr-N, Ti-Cr-N-Ni and Ti-Cr-Mo-N-Ni systems prepared by the arv-PVD method were studied.

The complete dissolution of TiN-CrN nitrides leads to the formation of a columnar structure with a grain diameter of about 500 nm. Layer-by-layer deposition leads to the formation of a series of alternating nitrides $Ti_xCr_{1-x}N$. At room temperature, such coatings demonstrate high physical and mechanical properties (hardness 32 GPa, wear resistanct $1.2 \cdot 10^{-5}$ $mm^3/(mm \cdot N)$. However, upon heating, as a result of the mutual dissolution of nitrides in each other, degradation of the polycrystalline nanostructure occurs with the formation of coarse grains. The addition of nickel to the Ti-Cr-Ni-N system leads to the formation of a polycrystalline structure. This is due to the fact that nickel, segregating at the boundaries of growing grains, prevents their growth. The coatings of this system are sensitive to nickel concentration, at a concentration of 0.2 at. % the hardness is about 42 GPa due to high macrostresses. An increase in the concentration of nickel over 3 at. % leads to a decrease in hardness less than 30 GPa. At the same time, coatings with a high concentration of nickel are characterized by lower wear resistance (about 10^{-6} $mm^3/(mm \cdot N)$. What is caused by the plastic extrusion of nickel, coatings with a low concentration, although they are characterized by wear resistance of the order of 10^{-5} $mm^3/(mm \cdot N)$, all the less during annealing because of relaxation of macrostresses, the decomposition of solid solutions and degradation of the structure occurs.

The coatings of the Ti-Cr-Mo-Ni-N system behave differently: because of a decrease in the concentration of titanium in the coating, the homologous temperature of the process increases. Consequently, the diffusion mobility of atoms on the surface and in the volume of the growing coating increases. This leads to the formation of a dense layered unstressed polycrystalline structure with a layer thickness of 1 to 24 nm. The configuration of the cathode system during deposition was such that nickel is located only in the layers enriched in titanium and molybdenium. After annealing, these layers retain their structure. While the chromium-rich and nickel-free layers recrystallize to form a monolayer. Despite these structural transformations, the physicomechanical and tribological properties when heated correspond to those of room temperature. In addition, molybdenum reduces the friction coefficient from 0.6 to 0.42 when heated.

Also, for all series of coatings, it was found that at a Ti more than 17 at. % and Cr less than 20 at. % the coatings are characterized by low oxidation resistance as a result of the formation of the Ti_2O_3 phase on the coating surface.

The financial support by the Russian Science Foundation Program (Research Project No. 19-19- 00555) is gratefully acknowledged.

Keywords: arc-PVD, nitrides, thermal stability, ceramics, coatings, thin films, wear

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Synthesis of $Ca_{n+1}Mn_nO_{3n+1}$ thin films by Pulsed-Laser Deposition

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Abstract:

Room temperature magnetoelectric (ME) compounds are rare and high-quality artificially multilayered ones are in general difficult and costly to produce. In this respect, magnetic Naturally Layered Perovskite structures (NLP) with improper ferroelectricity [1, 2], such as the Ruddleden-Popper calcium manganite compound $Ca_3Mn_2O_7$ [2], offer an alternative route to achieve non-expensive and high-performance room temperature MEs for information storage, sensors, and actuators or low power energy-efficient electronics. They allow exploring oxygen octahedra rotations and cation site to attain non-centrosymmetry. Additionally, due to their high sensitivity to lattice-distortions, their preparation in thin film form over crystalline substrates allows the manipulation of acentricity and adjusting of lattice, electric and magnetic interactions. However, for achieving this, the preparation conditions to obtain the envisaged $Ca_{n+1}Mn_nO_{3n+1}$ phases, with different n, need to be optimized.

Thus, here, thin films of calcium manganate have been prepared by laser ablation with different oxygen pressures (from 10^{-3} mbar to 10^{-1} mbar), substrate temperatures (from room temperature to 730 ºC), laser fluences (1-5 J/cm^2) and different substrates ($SrTiO_3$ and Si). The objective is to study the deposition conditions that lead to phase separated films, $Ca_{n+1}Mn_nO_{3n+1}$ with n = 1 ($CaMnO_3$), in particular, the improper ferroelectric $Ca_2Mn_3O_7$ (n = 2). Their structure was studied by X-ray diffraction (XRD). Their microstructure and morphology were examined by scanning electron microscopy (SEM), their chemistry was analyzed with energy-dispersive X-ray spectroscopy (EDS) and their magnetic properties were measured with a SQUID magnetometer.

The X-ray diffraction results show that for oxygen pressures in the range 10^{-2} - 10^{-1} mbar, deposition temperatures of 600 ºC to 730 ºC and laser fluences from 1.7 J/cm^2 to 2.9 J/cm^2, the films are polycrystalline, stabilizing in the $CaMnO_3$ (n = 1) orthorhombic Pnma phase. The SEM measurements show dense films with smooth surfaces. The corresponding EDS measurements indicate a 1:1 atomic proportion in these samples. On the other hand, by decreasing the oxygen pressure, increasing the temperature and increasing the laser fluence, the Ca/Mn proportion increases, so that for films prepared on $SrTiO_3$, at 730 ºC, with 4 J/cm^2 laser fluence and ~10^{-3} mbar oxygen pressure, the $Ca_2Mn_3O_7$ (n = 2) phase is stabilized, as confirmed by XRD. The corresponding EDS analysis further gives a Ca/Mn atomic ratio of ~1.4-1.5:1, consistent with the presence of this phase.

The corresponding magnetic properties of the films, that are correlated with their stabilized phases and preparation conditions, will be presented.

Keywords: Naturally Layered Perovskites, Ruddlesdon-Popper, Calcium manganese oxide, Thin films, Laser Ablation, Structural properties, Morphology, Magnetic properties

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Using 1D nanoimprint master templates to fabricate variable 2D nanogratings in indium tin oxide

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Abstract:

Specifically designed periodic nanostructures can be used to increase the performance of opto-electronic devices such as (O)LEDs or (O)PV as well as act as sensory surfaces in miniaturized sensor systems.[1,2] To be suitable for industrial application, the fabrication of these nanostructures must be feasible in a large-scale and low-cost process, which excludes commonly employed, highly controllable methods such as electron beam lithography and laser interference lithography. Nanoimprint lithography on the other hand enables high-throughput reproduction of multiscale structures,[3] but is restricted to the geometrical shape and dimensions of the employed master template. In this work we show the nanopatterning of a transparent conductive indium tin oxide (ITO) film employing UV nanoimprint lithography (UV-NIL) and ion beam etching (IBE). We are able to introduce periodic 2-dimensional (2D) nanogratings with variable grating depths and shapes into the ITO layer using only a single 1-dimensional (1D) master structure as an imprint stamp. In contrast to other works[4] we perform multiple subsequent steps of UV-NIL and IBE to preserve conformity to the original imprint template and control structural parameters for each of the two grating dimensions individually. We then use the resulting ITO nanogratings as a new master template for high-throughput replication of the desired greyscale 2D nanostructure. As ITO is a commonly used electrode material due to its favourable optical and electrical properties, the process is also suitable to provide nanostructured substrates for various thin film optoelectronic devices.

The authors acknowledge support by Interreg (Project Rollflex, 1_11.12.2014).

Keywords: nanoimprint lithography, ion beam etching, greyscale lithography, photonic crystal slab, periodic nanogratings, OLEDs, LEDs

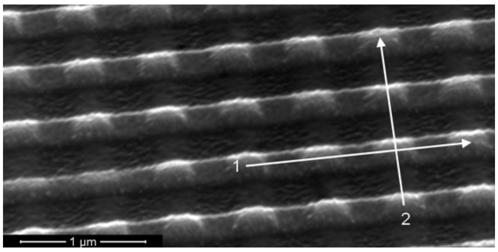

Figure 1: SEM image of the fabricated 2D nanograting in ITO showing the different grating depths along grating directions 1 and 2.

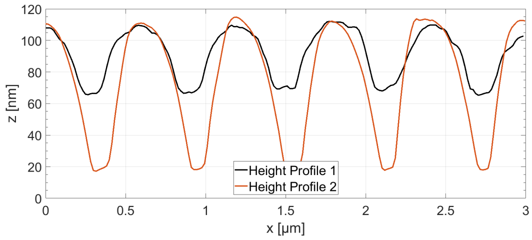

Figure 2: Height profiles of the fabricated 2D nanograting with 600 nm period in ITO along grating directions 1 and 2 measured by AFM.

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Thermal Laser Epitaxy – Ultrapure Epitaxy beyond PLD and MBE

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Abstract:

In oxide epitaxy, MBE is generally regarded as the method producing the highest quality heterostructures. To address new opportunities in adsorption-limited deposition, however, higher substrate and source temperatures are required, together with higher active oxygen background pressures. We explore cw laser heating for both the substrate and individual elemental sources to overcome these limitations. In such a system, shown in Fig. a), a long wavelength infrared laser is used to directly heat oxide substrates that are transparent to the radiation of standard heaters, allowing ultrahigh substrate temperatures above 2000 °C. Most elements in the periodic table are metals with melting points in or even above the range of fluxes required for deposition. Under these conditions, heating the central region of a source target by a laser produces temperature gradients large enough so that the target does not melt as a whole, as demonstrated for a 12 mm diameter Si source in Fig. b). All these materials can therefore be evaporated without crucibles, by merely suspending them between three support points.

Using a working distance of 60 mm, we achieve growth rates of more than 1 Å/s. We have experimentally verified such crucible-free evaporation (Fig. b)) already for a majority of the non-radioactive elements in the periodic table (Fig. d)).

A thermal laser epitaxy (TLE) system based on this laser only approach (Fig. a)) offers a number of advantages. As there are no filaments or other corrosion sensitive parts in the chamber, the background pressure is limited only by the mean free path not dropping below the source-sample distance. Reliable deposition is possible in up to 10^{-2} hPa ozone/oxygen, such as during the growth of the oxide layer shown in Fig. c). As there are no hot filaments in the vacuum, both highly corrosive background gases and ultra-pure operation are possible. We measure chamber pressures of 6×10^{-11} hPa at substrate temperatures of 1400 °C and 2×10^{-10} hPa during the deposition of Ru at a rate of 0.2 Å/s. The source targets are transferable in the same way as the substrates, allowing a flexible operation with different source materials in subsequent runs. The small source targets enable short working distances, allowing an efficient use of the source material, e.g. when working with expensive rare materials. The same scaling arguments as in MBE apply, permitting a straightforward upscaling of the epitaxy process to large substrate sizes. The process is agile, the substrate and the sources can be ramped at extreme rates due to their small heat capacity with direct heating and the absence of crucibles and the associated thermal expansion mismatch problems, thereby allowing high throughput volumes. And finally, the process chamber can be very small and simple, allowing both long uptimes and fast and easy rebuild or replacement in case of contamination or damage.

Keywords: epitaxy, laser, deposition, molecular beam epitaxy, pulsed laser deposition, oxides, thin films.

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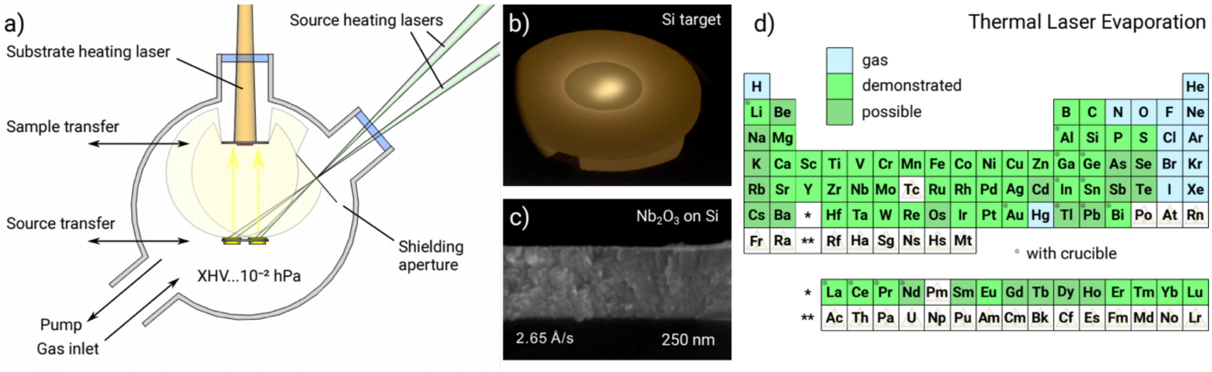

Spectroscopic ellipsometry studies on solution processed OLED devices: optical properties and interfacial layers

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Abstract:

The fabrication of efficient organic light emitting diodes (OLEDs) in large volume production by solution based roll-to-roll manufacturing technologies is of high scientific and technological interest. These devices contain many layers of different functionality like hole injection layer (HIL), emissive layer (EML), electron transport layer (ETL) apart from electrodes. However, the fabrication of these multilayers from solution involves the major problem of stack integrity due to the fact that the sequential layers are soluble in common organic solvents. Thus, the composition and the characteristics of the resulting interfaces of solution-processed layers are critical factors in determining device performance. This work deals with the NIR-Vis-Far UV Spectroscopic Ellipsometry (SE) characterization of polyfluorene-based OLED devices. Poly(9,9-dioctylfluorene) (F8) and poly(9,9-dioctylfluorene-alt-benzothiadiazole) (F8BT) is used as an EML in the OLEDs. The HIL, EML and ETL layers have been developed using the slot-die process, onto indium tin oxide (ITO) coated polyethylene terephthalate (PET) flexible substrates, under ambient conditions. The SE data are analyzed using: (i) the modified Tauc–Lorentz (TL) dispersion model, in which the energy-depended broadening of the TL oscillator is introduced, in order to interpret the optical dielectric response of each material, (ii) the Effective Medium Approximation (EMA) for the investigation of the interfaces' characteristics, and (iii) the appropriate geometrical model for the description of the multilayer OLED structure. The results highlight the degree of intermixing within the layers and provide information about the interfaces and they are correlated with the emission characteristics as well as the final performance of the OLED devices.

Keywords: F8:F8BT, OLED devices, Ellipsometry, slot-die, printing, green emission, polymer blend.

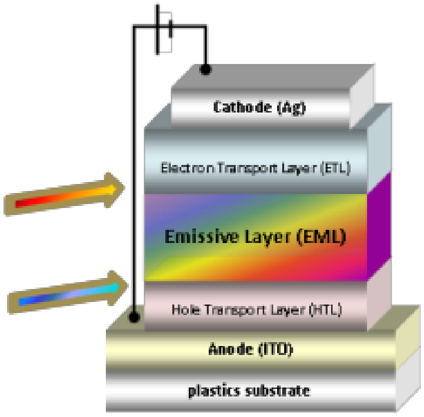

Figure 1: The multilayer OLED structures, with solution processed HTL, EML and ETL layers. Arrows denote the critical interfaces studied in this work using Spectroscopic Ellipsometry.

Acknowledgments:

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

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Preparation of High Density Polyurethane Surfaces for Metallization

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Abstract:
Commercial polyurethanes (PU) are electrically insulating materials and durable at high temperatures. Although, the high density PU used in this study has relatively higher electrical conductivity (2.2 Ωm) and low thermal expansion coefficient ($15*10^{-6}$ K^{-1}), surface metallization was necessary for subsequent electroplating processes. The surface metallization was carried out by multi-step processes which included degreasing, etching, sensitization, activation and electroless nickel plating. In the case of sensitization by tin, the complex colloids of an Sn sensitization solution consist primarily of Sn^{4+} cores were stabilized by Sn^{2+} outer layer. The diameters of these colloids were approximately 25 to 100 Å. After sensitization, the surface was metallized with Pd by oxidizing the Sn^{2+} to Sn^{4+} and reducing Pd^{2+} ions to Pd atoms using an activation solution. Surfaces were characterized for surface morphology, roughness and physical properties at different stages of metallization. The results showed that surface sensitization and activation processes increased the surface conductivity of the foam. The surface morphology indicated the presence of Pd nuclei on the surface after the activation process. Electroless Ni plating increased the thickness of the metallized surface. Possible aerospace applications of the coating technique developed includes a new generation of tooling devices for nanocomposites.

Keywords: surface metallization, electroless nickel plating, surface sensitization, surface activation, aerospace, nano-sized surface sensitization.

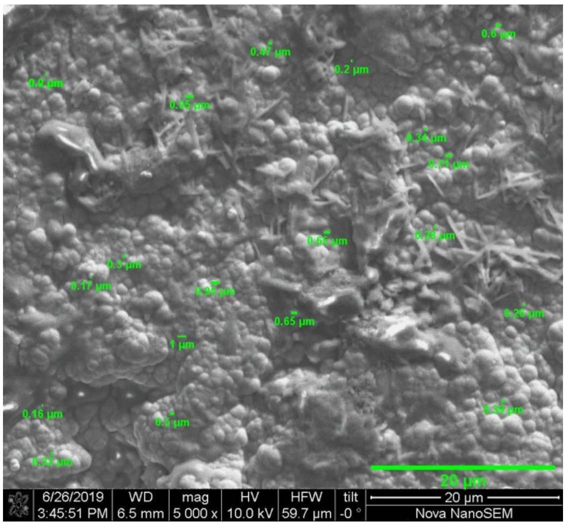

Figure 1: An image illustrating the high density polyurethane surface after the sensitization, activation and electroless nickel plating processes.

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Nanotech / Nanometrology Session II. B: Nanomaterials Modelling and Characterisation

How can we “see” and “feel” the dynamics at nanoscale: A scanning probe microscope approach

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Mechanical & Aerospace Engineering, Rutgers University, USA

Abstract:

Scanning probe microscope (SPM) has become the enabling tool for us to “to image, characterize, modify, and manipulate a wide spectrum of materials at nano- to atomic scale. Although throughout these years we have witnesses significant improvements of SPM technologies, currently SPM still comes short in capturing and measuring nanoscale dynamic processes, particularly when the dynamic processes are occurring rapidly in minutes or even faster, over a relatively large area of tens of micrometers or even larger, and in soft samples of dedicated surface such as live mammalian cells. Such a limitation is largely due to the challenges in addressing the issues caused by the excitation of the intertwined dynamics and hysteresis effects of piezoelectric actuators, the nonlinear probe-sample interaction dynamics, the distributive hydrodynamic disturbance force, and the need of applied force to rapidly excite the material properties (not others). In this talk, I will present a suite of SPM imaging and mechanical mapping tools recently developed by our group for high-speed SPM imaging, rapid broadband nanomechanical quantifications and rapid simultaneous imaging and broadband nanomechanical mapping of soft materials. Experimental examples on polymer samples and live cells will be presented and discussed.

Manufacture and calibration of high stiffness AFM cantilevers

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Abstract:

Atomic force microscopy (AFM) employs microfabricated cantilevers as sensing elements, which are used to measure surface topography and interaction forces. The flexible free end of a cantilever often presents either a pyramidal tip or a colloid probe particle. Cantilevers are traditionally V-shaped or rectangular, and are generally fabricated from Si or Si_xN_y. Laser light is reflected off the free end of the cantilever onto a position-sensitive photodetector (PSD). AFM force measurement studies began in earnest during the early 1990s, followed by significant efforts to accurately calibrate the mechanical properties of the cantilever. These efforts centred on understanding the beam mechanics, in particular the flexibility of the free end, where the tip or colloid probe is situated.

Force measurements have been applied to a wide variety of scientific and engineering disciplines, and across many industrial sectors. For many studies, the use of colloid probes or chemical functionalisation permits the selective study of a particular material/material interaction, often under non-ambient environments. Force measurements can provide information regarding sample mechanical properties, during the tip/sample approach, as well as adhesive properties, during the tip/sample separation. The spring constant is a measure of the cantilever stiffness, i.e. the resistance to bending. The spring constant of a rectangular cantilever can be estimated using Euler-Bernoulli beam theory. Once calibrated, the spring constant is used in calculations in order to convert normal (i.e. vertical) deflections into normal forces using Hooke's law.

The range of AFM cantilevers commercially manufactured means that spring constants in the approximate range 10^{-3} to 10^{2} N m^{-1} are available. Deflections in the range 0.1-100 nm are typically measurable on the PSD, and hence forces can be measured in the picoNewton (10^{-12} N) to microNewton (10^{-6} N) range. Accurate control of the beam thickness during fabrication is particularly difficult to achieve, due to the nature of the etching process employed. The width and length of the beam are generally much more reliable and repeatable. Given the sensitivity of the spring constant to the beam thickness, typically proportional to $(\text{thickness})^3$, accurate calibration is a necessity for accurate force measurements.

We are currently calibrating 40 different designs of rectangular AFM cantilever, designed using Timoshenko beam theory, manufactured from Si. The various designs incorporate a range of widths, lengths, and thicknesses. These cantilevers are expected to exhibit spring constants in the range 10^{2} to 10^{5} N m^{-1}. This would afford researchers the opportunity to perform adhesion, indentation, and tribological testing with normal loads approaching 1 mN, whilst retaining the displacement resolution of the AFM. We present the latest results of this project, including measured cantilever resonant frequencies and calculated spring constants, which are compared to analytic expressions and finite element models.

Keywords

adhesion, beam, cantilever, force, friction, load, spring constant, stiffness, tribology

Nanoscale monitoring of the molecular complexes structural and mechanical changes by use of the AFM

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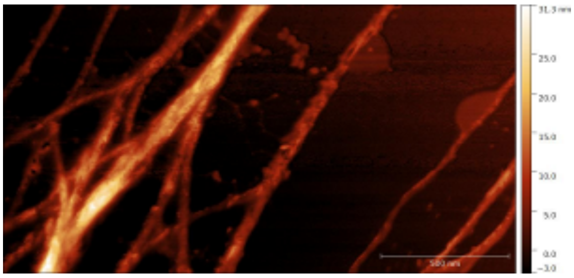
Abstract:
The last three decades have brought a critical improvement into the field of microscopy and proteomics; correlations between the shapes of microscopic structures and their function were revealed. However, the structure of the biomolecules is not the only parameter determining the physiological function. However, also other parameters, such as composition, charge location, and mechanical properties, are essential to understand the behaviour of biomolecules and their complexes. Mechanobiology brings together various scientific disciplines, thus helps to characterize how the protein molecules, cells, and tissues respond to mechanical cues that contribute to differentiation, development, structural and disease processes. Atomic force microscopy (AFM) has grown from the solid material characterization method to a critical device allowing the simultaneous topographical and mechanical characterization of living biological systems.

The ability of the AFM to study biomolecular assemblies will be illustrated in various examples. This method was used to support studies of myeloperoxidase-mediated alteration of endothelial function via complex formation with hyaluronan (Figure 1), encapsulation of the enzyme inhibitors into the ferritin cage, and to study the structure and mechanical properties of polyglutamine nuclear complexes closely connected with the CAG repeat neurodegenerative disorders.

Keywords: atomic force microscopy, biomolecules, biomechanics, nanostructure



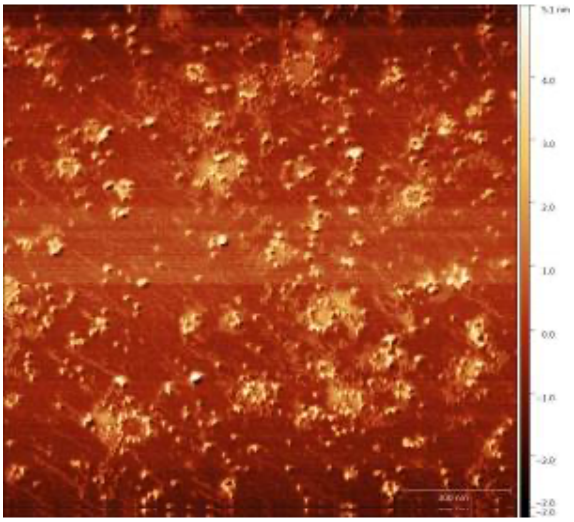


Figure 1: Figure illustrates the ability of the AFM microscopy to investigate the structure of hyaluronan biomolecule in a nanoscale (upper image) and its complex with molecules of myeloperoxidase (lower image).

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SiC Nanowire Foams for pressure detection

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Abstract:

Using carbon nanotube or graphene-based nanocomposites as electromechanical sensors has been well-studied, however their relatively poor stiffness, low chemical inertness and thermal insulation effect of such carbon materials have limited their utilisation under harsh conditions (e.g. high temperature, corrosive etc.). In this context, we will present a SiC nanowire (SiCNW) foam to counter these deficiencies of carbon-based materials. We will demonstrate that the electric resistance of the SiC ceramic-based foam, prepared by a carbothermal reduction of SiO_2 using kitchen sugar, responses rapidly to compressive pressures.

The resultant foam, possessing a high overall porosity of ~96%, exhibited a two region character, representing a bulk core-shell structure. The fluffy shell layer consists of numerous smooth and long SiC nanowires, wrapping the core part which constitutes short SiC whiskers mixed with a small amount of SiC flakes. The foams showed good recoverability under compression load at a strain of $\varepsilon = 20\%$, and high structural robustness with a compressive modulus up to ~1.35 MPa, which is slightly higher than existing carbon nanotubes/graphene sponges of similar densities. Existing pressure detectors are mainly designed for finger force detection, whilst the present SiC nanowire foams are capable of detecting large dynamic compressive loads, ranging 130~651 kPa. The present foams offer stable and drift-free resistance responses from 500 to 1000 Ω, which is 500 times wider than that of carbon-polymer composite sensors.

These light-weight, highly porous, compressible, and thermally stable features of the SiC nanowire foams are promising for applications in electromechanical micro-devices (MEMS) to monitor vibration, acoustic, and structural damages.

Keywords: carbothermal reduction, SiC nanowire, SiC foam, pressure detector, thermal insulation

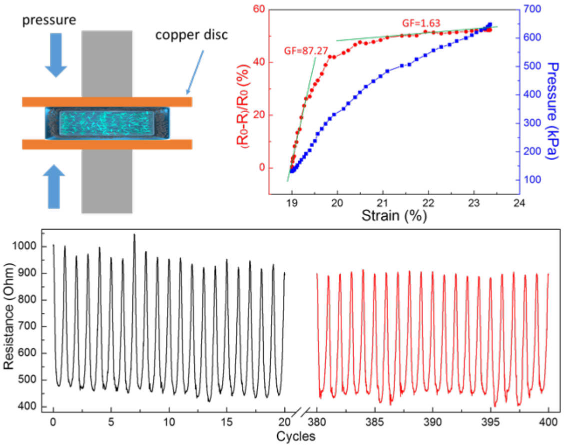

Figure 1: An illustration of the electrical resistance testing of the core-shell SiCNW foam at different compressing cycles, up to 400 cycles measured.

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In situ generation of sub-10 nm silver nanowires under electron beam irradiation in a TEM

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Abstract:

Sub-10 nm quasi-one dimensional (1D) nanostructures have received increasing interest for their use as small basic building units in nanodevices. One dimensional Silver (Ag) nanostructures, as one of the promising candidates for electronics, plasmonics and sensing applications, have been fabricated by a variety of chemical and physical strategies. However, preparing sub-10 nm (diameter) 1D Ag nanostructures for nanofabrication remains challenging experimentally and the nucleation and growth dynamics of the Ag nanowires are still not fully understood (1-4).

In this work, we report the segregation-driven in situ generation of Ag NWs on the surface of a Ag_2WO_4 (AWO) nanorod (NR) under electron beam irradiation in an aberration corrected-TEM (AC-TEM). We adopted AWO as the starting material because previous studies have demonstrated Ag surface segregation and the formation of Ag NPs on the oxide support under plasma or electron beam irradiation (5-7). By controlling the electron irradiation dose rate, sub-10 nm Ag NWs (9.5 ± 0.2 nm) are fabricated on the oxide surface. The generated Ag NWs show a tunable length/diameter aspect ratio, and the formed surface in the NWs is the low-energy {111} plane. The direct in situ observations on the nucleation and growth dynamics uncover that the sub-10 nm silver NWs show a combined growth process of linear first-order kinetics and nonlinear second order kinetics in the lateral direction and the electron dose rate plays an important role in regulating the diameter of the supported Ag NWs (8). The ability to fabricate Ag NWs in a controllable way by using electron beam irradiation represents a significant step forward to the further applications of Ag NWs in nanodevices. The present study opens a new avenue for the fabrication of supported sub-10 nm Ag nanowires through an electron beam irradiation nanofabrication route and highlights the importance of irradiation dose- and dynamics controlled materials growth.

Keywords: 1D Nanostructures, In situ TEM, Ag Nanowires, electron beam irradiation, nucleation, growth dynamics, nanofabrication.

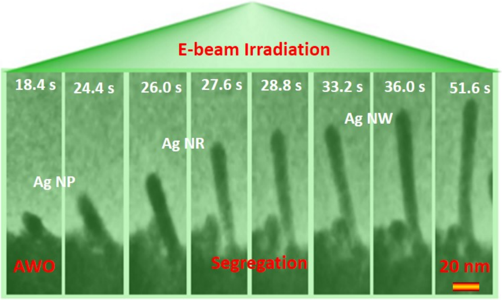

Figure 1: Ag nanowires fabricated on Ag_2WO_4 support based on a segregation driven growth route under electron beam irradiation within the TEM.

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Challenges on inline monitoring of nanosized polymer materials

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Abstract:

Inline monitoring of production processes at industrially relevant properties is a highly challenging topic in research and industry application. Due to high volume fractions, high turbidity and dependend scattering inline monitoring of dispersions is still a great challenge. Photon Density Wave (PDW) spectroscopy is a novel measurement technique for the independent determination of the absorption coefficient μ_a and the reduced scattering coefficient μ_s' of highly turbid samples. In contrast to most analytical methods commonly used in inline process analytics, PDW spectroscopy does not saturate at high volume fractions and is applicable for inline measurements both in industrial applications and scientific research [1]. Example applications are in food, cosmetics, paint and coatings industry. PDW spectroscopy is applied to access the chemical as well as physical properties, such as particle size, volume fraction or absorption of nanosized materials in dispersions.

PDW spectroscopy uses intensity modulated laser light, transported via optical fibers into samples with volume fractions up to 50 wt-% of scattering material [2]. Inline measurements are achieved using a small diameter probe, which is robust against fouling and allows for non-destructive analysis during the process directly through a reactor inlet. The direct inlet of the probe guarantees real-time access to multiple process parameters.

This talk will give insights into PDW spectroscopy and its applications, especially in nanoscale polymer chemistry. The monitoring of different polymer syntheses and inline particle growth is presented. This enables process control on final particle size, particle size distribution and properties of the product. Latest research showed, that analysing polyvinyl acetate particles regarding their particle size is challenging, due to the complex sample composition.The study shows very good agreement of inline, dilution-free obtained particle size resulting from PDW spectroscopy and offline dilution based light scattering techniques and optical imaging.

Keywords: inline monitoring, polymer synthesis, Photon Density Wave spectroscopy, particle size analysis, particle size distribution.

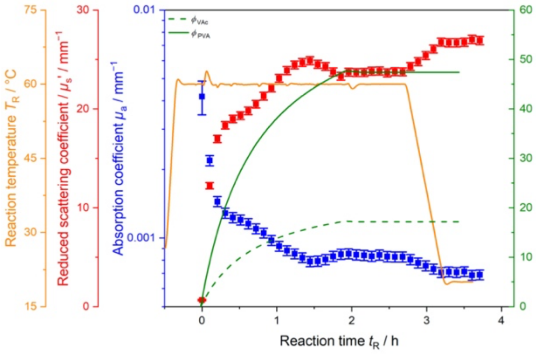

Figure 1: Inline monitoring of polyvinyl acetate synthesis using PDW spectroscopy as tool to access the scattering (red) and absorption (blue) properties of nanometer sized polymers in dispersion [3].

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Comb-referenced interferometry in nanopositioning and nanomeasuring machines

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Abstract:

The increasing impact of nanofabrication techniques in research and industry requires high performance distance measurement and positioning systems to provide resolving capabilities down to the sub-nm-range over several hundred millimeters of measurement range. In recent years the next generation of the nanopositioning and measuring machine (NPMM) was developed at the TU Ilmenau. The NPMM-200 currently provides a measuring range of 200 mm x 200 mm x 25 mm at a resolution of 20 pm and a measuring reproducibility of 80 pm [1]. This performance also sets new demands on the frequency stability of the He-Ne lasers and their corresponding wavelength used as a measuring standard in the underlying fiber-coupled laser interferometers. Currently their longterm frequency stability is limited to $2\cdot10^{-9}$ [2].

In this study we report the approach of directly stabilizing the He-Ne lasers of the NPMM-200 to a single teeth of an optical frequency comb (OFC). The comb itself is referenced to a GPS disciplined oscillator providing a relative Allan deviation better than $4\cdot10^{-12}$ (1s) [2]. This way a permantent link between laser frequency and the frequency of an atomic clock is created allowing a direct traceability to the SI definition of time.The transfer regime is depicted in Fig. 1.

We will present the stabilization regime allowing us to transfer the stability onto the metrology lasers of the NPMM with a relative Allan deviation better than $6\cdot10^{-13}$ (1s) [2,3]. We will discuss the impact of distortions on the short- and longterm frequency stability of our transfer configuration and demonstrate the influence of frequency stability on the interferometric length measurement in the NPMM-200.

Keywords: nanometrology, optical frequency comb, laser interferometer, laser stabilization

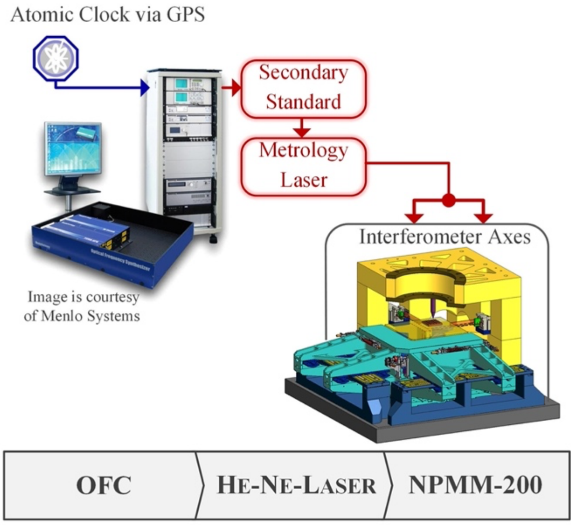

Figure 1: Providing a permanent link between an atomic clock and the metrology lasers of the NPMM-200 by means of an optical frequency comb.

References:

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Nanoplastics characterization at the biological interface

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Abstract:
Plastic pollution is a great issue affecting our Planet, especially marine ecosystems. Once enter the environment, plastics undergo degradation processes and fragment into smaller pieces up to the nanoscale. Damages caused by large plastic items to marine organisms are well known, but micro- and nanoplastics could be even more dangerous. These nanoparticles can enter the organisms, penetrate tissues and biological barriers and can interact with cells and biological molecules[1]. Unfortunately, the small size of these pollutants makes their isolation from the environment difficult, and this fact also strongly hampers their characterization. There is an urgent need for the creation of reference materials that better reflect the real characteristics of nanoplastics naturally form in the environment, like the heterogeneity in size, shape, surface and composition. In this work, we present a study on the production, isolation and characterization of nanoplastics. Starting from commonly used disposable plastic items, we used mechanical disruption to fragment macro-pieces into nanoplastics in a controlled way. After a concentration step by centrifugation, we used consolidated techniques in the field of nanomaterials, such as scanning probe microscopy, size distribution and spectroscopic characterization techniques, to provide a fingerprint and a quantification of nanoplastics. We also present a preliminary study on the interaction of nanoplastics with biological fluids and the formation and characterization of the protein corona.

Keywords: nanoplastics, characterization, reference material, protein corona, biological interface, nanotoxicity.

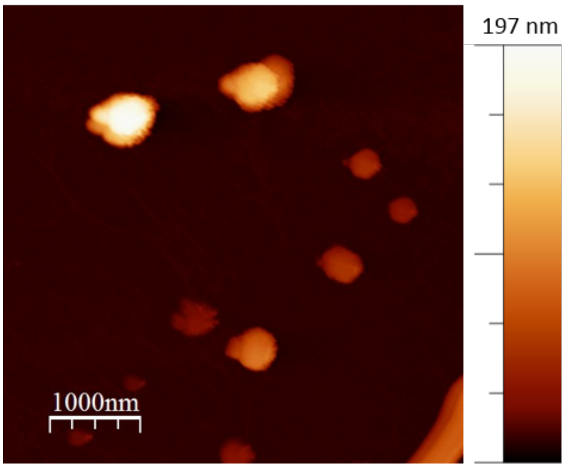

Figure 1: Figure illustrating a sample of nanoplastics produced by mechanical fragmentation and characterized by Atomic Force Microscopy.

References:

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Disease Control via Mosquito Nano-Tech-Repellents

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Abstract:

COST Action CA16227 is entitled Investigation and Mathematical Analysis of Avant-garde Disease Control via Mosquito Nano-Tech-Repellents. Some of the control measures involve new technologies in textile and paint products based on nano- and micro-particles releasing repellents or pesticides in well portioned dosages. Another control measure is the use of thin layers of graphene in clothing through which mosquitos cannot bite and a graphene-polymer through which chemical signals from the body that encourage mosquitos to bite cannot pass.

We will report on all of these measures and their efficacies. For example, the polymer used is a PVDF (poly (vinylidene fluoride)) matrix reinforced with graphene. We present the tensile strength of this material as compared to the force of mosquito bites. The repellents used are microencapsulations of essential oils (Immortelle and Litsea, e.g.). In one study the repellency was 100%.

The proposer is a member of the Management Committee (MC) of this Action from Malta and is part of the Mathematical Analysis, Data Analysis and Statistics working group. Work on how to form regions for distribution of nano- or micro-encapsulatons of repellents or insecticides will also be exhibited.

Keywords: nano-particles; micro-particles; microencapsulation; mosquito control; vector borne diseases; essential oils; Graphene; Graphene Layers; Crystallite Size; Electrolysis; Reverse Voltage; electrochemical production; X-ray diffraction; convex regions; sectorization; territory design

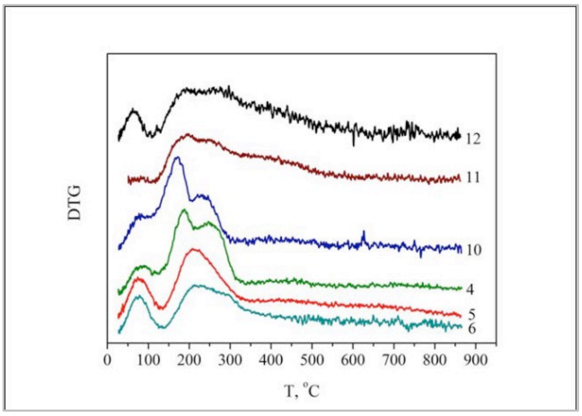

Figure 1: Thermal Diagrams of the Studied Graphene Samples: DTG Curves

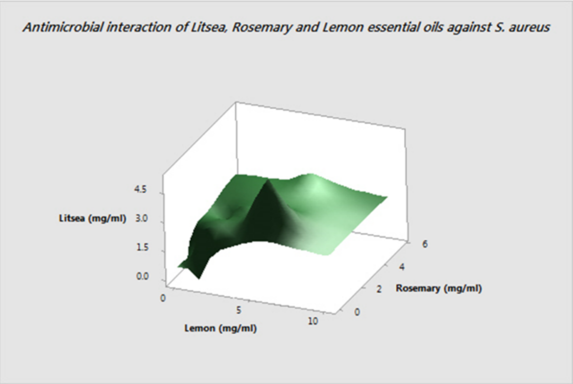

Figure 2

References:

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Molecular Dynamics of ion transport through SWCNTs: a focus on water model and pore geometrical parameter effects.

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Abstract:

Single-walled carbon nanotubes (SWNTs) have shown great potential for manufacturing nanofluidic devices capable of filtering solutions containing several types of ions to mimic biological membranes, harvesting energy by connecting electrolyte reservoirs at each side of the tube, sensing and controlling ion motion[1]… Broad area applications may emerge from such devices such as flow sensing, drug delivery, sea-water desalination and energy conversion[2].

During the past two decades, nanofluidic devices based on carbon nanotubes have been extensively studied experimentally and many curious phenomena have been observed such as high ionic conductance due to fast ion motion inside the pore and stochastic current behaviors.

In this work, the study of ionic transport in CNTs of small diameters through molecular dynamics provides additional information to experimental studies. The diameter and length of the CNT were modified to take into account the effect of the geometric parameters of the tube on the ionic conductance. On the other hand, a set of rigid and non-polarizable water models at three sites was selected in order to evaluate the water model effect on ionic conductance inside the SWCNT: TIP3P, SPC/E and TIP4/2005.

Keywords: nanofluidic devices, SWCNT, ion transport, water model.

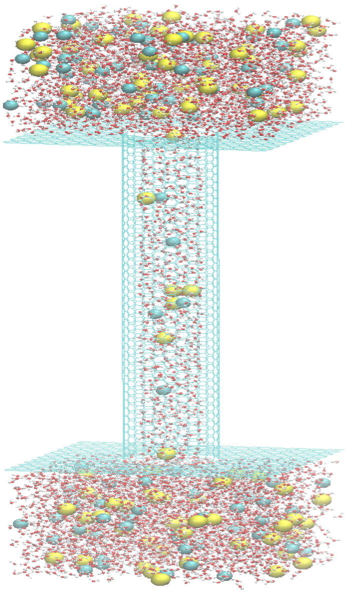

Figure 1: Ion transport inside carbon nanotube connecting two electrolyte reservoirs.

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Ring-o-rings: joining the ends of poly[M]-catenanes to control supra-molecular torsion

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[2] INFN-TIFPA, Trento, Italy
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Abstract:

Recent advancements in chemical synthesis and self-assembly as well as modelling and simulations have offered a framework to design systems of interlocked rings with controllable properties. These systems can be produced at scales varying from a few nanometers to several micrometers, and have been proposed for applications ranging from smart materials, to catalyzers and nano-machines. Of particular interest are poly[M]-catenanes, linear sequences of M mechanically interlocked circular molecules, which can be synthesised through self assembly. Most of the work so far has been focussed on the variety of features that the molecular mobility of the mechanical bond may confer to poly[M]-catenanes compared to standard polymers. Here we show that, by joining the two ends of a poly[M]-catenane to form a supramolecular ring, it is possible to capture different amount of torsion and hence alter significantly the average extension of the structure as well as local properties such as the relative orientation of the elementary rings along the backbone and their local density. Finally, by extending the notion of twist and writhe of ribbon-like structures to circular poly[M]-catenananes we show that their sum is, on average, conserved and equal to the number of elementary rings assembled to induce the desired amount of torsion. Our results indicate that versatile supramolecular structures can be designed in such a way to store a controlled amount of torsional stress, opening several potential applications for novel smart materials.

Keywords: catenanes, topology, rings, simulations, supramolecular chemistry, polymers

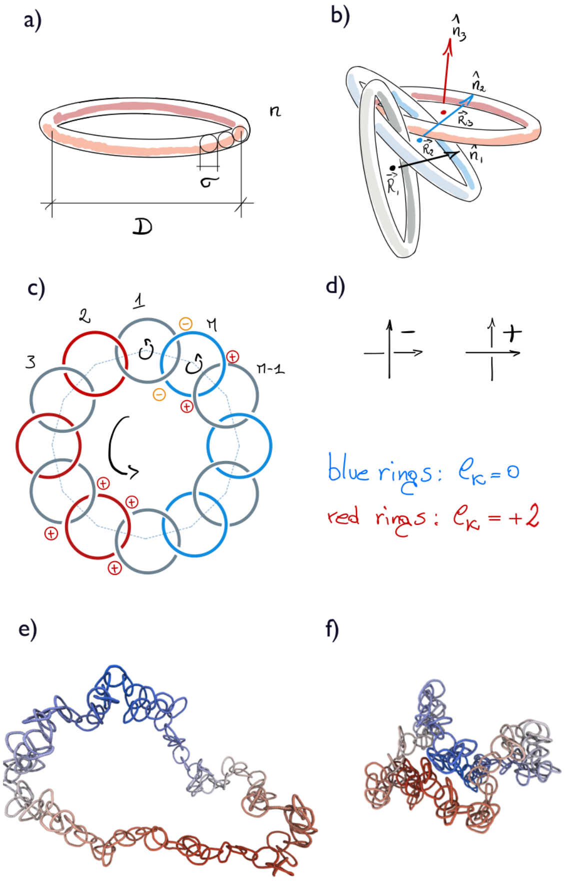

Figure 1: Systems studied. The simulated catenanes are composed of M rigid rings of thickness sigma and diameter D (a), topologically linked with each other to form a circular catenane (b), (c). The amount of stored torsion contained in the catenane can be controlled in the simulation by changing the twist inserted through linking (d). Different amount of stored torsion radically change the system behaviour, as shown by the snapshots in panels (e) - zero torsion - and (f) -maximum torsion.

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Experimental study of colloidal particles confined in a droplet formed in a microfluidic channel

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Abstract:

Particles are sometimes added during droplet formation to replace surfactants as surface active agents and improve the stability of the dispersions ([1]Ridel et al. (2016), [2]Albert et al. (2019)). Generally, it is assumed that these particles follow classic Brownian motion inside the droplets. But, as shown by [3]Ghosn et al. (2016), if the particles are confined their behaviour can be modified. This results was also observed numerically by [4]Li et al. (2021) for spherical and cylindrical particles inside a rigid spherical cavity. In recent years, microfluidics have been used extensively to produce dispersions with size distributions. However, the dynamics of confined particles in droplets formed in microfluidic channels is still poorly understood. In the present work, the displacement of particles inside a fixed droplet was investigated using fluorescently tagged 3 µm polystyrene particles (with an absorbance of 532 nm and an emission of 612 nm) illuminated by a continuous green laser. This setup allows to track both time and spatial evolution of the particles inside the droplet. The droplet phase was a glycerol/water solution and the outer phase was silicone oil. Experiments were carried out at different particle concentrations. Droplets were generated in a flow focusing glass microchannel (with width and depth of the main channel 390 µm and 190 µm respectively, 390 µm and 190 µm) and were trapped using a stop valve system. To follow the particles displacement, images were taken with a 16 bit high-resolution camera with 2048×2048 pixels resolution equipped with a 20× microscope lens. A green laser (532 nm) ensured a microchannel illumination. To eliminate light reflections, the lens was mounted with an orange filter. To capture the particles displacement over time, images were taken with a frequency of 4Hz. The trajectory of the particles were obtained to calculate both radial and azimuthal mean square displacement (MSD). The results showed that the MSD behaviour change significantly with the particles concentration and the radial location.

Keywords: microchannel, droplets, colloids, confinement effect, Brownian motion, interfacial tension.

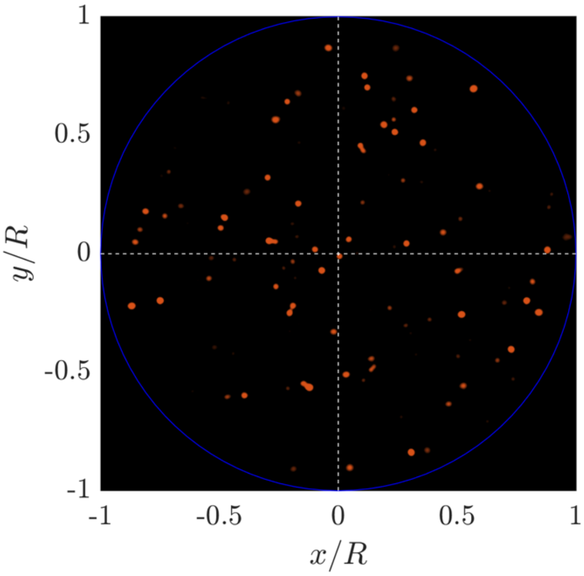

Figure 1: Visualisation of 3 µm polystyrene particles inside a droplet with a radius R = 120 µm. The blue line follow the droplet interface.

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The Effect of Particle Loading, Surfactant Concentration and Sonication Time on The Wettability Of Multi-Walled Carbon Nanotubes Based Nanofluid

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Abstract:

The wettability aspect of the multi-walled carbon nanotubes (MWCNTs) based nanofluid was investigated for different nanoparticle MWCNTs concentration, sonication times, and surfactant concentrations. The wettability was experimentally evaluated using the contact angle method based on L9OA orthogonal array. The analysis of variance (ANOVA) showed that the MWCNT loading is the most influential factor followed by surfactant concentration and sonication time, respectively. Besides, the contact angle was found to be increased with increasing the MWCNTs concentration. However, decreasing the surfactant concentration increases the contact angle. This study provides insights about the underlying physical mechanism of nanofluid wettability and makes progress towards solving the conflicting theories proposed in the open literature.

Keywords: nanofluids, MWCNTs, wettability, contact angle, mechanisms.

Colloidal Suspenssion of Silver Nanoparticles for Random Dispersion of LASER Beams

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Abstract:

The interaction of LASER beams with bacteria mixtures is a an area of scientific research with various applications in the field of biotechnologies, antibacterial protection, pharmaceutics and medicine in general. There are various situations of interactions with the need to assure focused or dispersed beams.

The proposed paper is synthetizing the results of the research project MULTISCALE – “Development of Advanced Materials by Integrating Nanomaterials and Nanotechnologies, Using Multiscale and Multiphysics Optimization, Dedicated to High-Performance Energy Systems” that is carried out in partnership between a University research group and industrial companies for innovative products and services. The grouping of industrial companies is including a manufacturer of high performance LASER systems and installation that have collaborated on the development and validation of a concept of biostimulation solutions of bacteria mixtures in anaerobic conditions using selected LASER beams.

The system is centered on the development of dispersor for large volume dispersion selected of LASER beams, using nanofluids with suspensions of silver nanoparticles. The dispersion properties of the device can be tuned based on the composition of the nanofluids and the appropriate selection of the size of silver nanoparticles.

Thre were tested several methods of synthesis of silver nanoparticles, stabilization solutions of nanofluids based on silver nanoparticles and the interaction between the LASER beams and the colloidal sustensions of nanoparticles.

The paper is synthesizing the research activities, the investigation methods and the experimental results obtained by the implementation of the project activities.

Keywords: silver nanoparticles, colloidal suspenssions of nanoparticles, nanofluids, LASER beams, LASER biostimulation, LASER beam scattering.

Figure 1: Experimental setup for the dispersion of LASER beams in a batch reactor with bacteria mxtures.

References:

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Nanotech / Biotech
Joint Session II. C

The interplay of efficiency and biodegradation for inorganic nanohybrids in cancer or regenerative therapies.

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Abstract:
The emergence of multifunctional inorganic nanohybrids providing multiples functions recently paved the way to tailor-made therapeutic prescriptions and theranostic functionalities.

In cancer therapy, they have raised the prospect of thermal treatments that have few if any adverse effects. We recently compared the heating potential of magnetic nanoparticles under magnetic hyperthermia or photothermia[1,2], of plasmonic nanoparticles under photothermia[3], or the combination of both[4-8], towards synergistic solutions to complete cancer cell destruction. Different pre-clinical studies will be showcased, exploring in vivo these nanoparticles-based modalities. Among others, will be discussed - nanohybrids featuring a magnetic core and a copper sulfide shell to perform all at once magnetic hyperthermia, photothermal therapy and photodynamic therapy; - nanohybrids combining two plasmonic materials, to enhance the photo-thermal potential of each; - biosynthesized magnetosomes combined with a genetically encoded targeting unit in order to achieve enhanced photothermal treatment following intravenous injection.

The magnetism of iron oxide - based nanomaterials also provide cells with sufficient magnetization to manipulate them. Magnetic nanoparticles thus appear as a promising tool for tissue engineering opening up challenging perspectives. We developed magnetic-based methods to manipulate cells, towards the goal to provide magnetic artificial tissue replacements[9,10,11,12], that can be stimulated on demand, for instance to induce mechanically stem cells differentiation[13,14].

The therapeutic use of nanoparticles in cancer therapy or regenerative medicine application still raises the more general issue of intracellular nanoparticle long-term fate[15]. Cell spheroids models and magneto-thermal tools will be introduced, as tools to monitor long-term nanomaterials intracellular integrity. It evidenced a massive intracellular degradation[16], which could be prevented by a polymeric coating[17] or an inert gold shell[18,19]. Remarkably, human cells could also biosynthesize their own nanoparticles, from the intracellular degradation products of synthetic ones[20,21,22], with longer persistence, and limited toxicity.

Keywords: Magnetic and Plasmonic Nanoparticles, Biodegradation, Biocompatibility, Bioprocessing, Photothermia, Magnetic Hyperthermia, Tissue Engineering, Biophysical Cell Stimulations.

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22. ACS nano 10.1021/acsnano.1c00567 (2021)

Fundamental Chronobiological Changes in Nanostructure of Bone Tissue

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Abstract:
Mechanisms resulting in age-related and pathology-induced changes in nanostructure and molecular dynamics in bone are investigated by combining X-ray diffraction, Raman scattering, IR and X-ray absorption spectroscopy and inner-shell photoemission. Cortical bone of newborn, adult and mature health rats is used as object to study general regularities of age-dependent phenomena. Medial and lateral condyles of the femur resected during total knee arthroplasty in patients with medial compartmental knee osteoarthritis (OA) are used as samples to understand pathology induced chronobiological (intact → partially → completely damaged cartillage) changes in local electronic and atomic structure of femoral bone [1]. Analyzing the experimental data and applying the 3DSL model [2] we (i) extract the age- and site-dependent deviations of the spectroscopic and structural characteristics of mineralized bone, (ii) examine relationships between nanostructure and hierarchical organization of the skeleton, (iii) reveal the chrobiological changes at the subcellular level. Figure 1 illustrates the chrobiological changes in the Ca and P 2p binding energies (solid lines), crystallinity (yellow diagram) and lattice constants ***a*** and ***c*** (dashed lines) of hydroxyapatite crystallographic cell. The chronobiology in OA-damaged areas is found closely related with forming non-apatite chemical bonds [1]. It is shown that dominant role of apatite Ca^{2+} states in bone is an indicator of its health [1]. The site-depent density of the apatite states in OA areas is exhibited with blue diagram in Figure 1. Inspecting the Ca^{2+} 2p photoemission spectra we approximate the Ca 2p BE as an exponential function of the ratio of age t to life expectancy $\langle T \rangle$. The substantially different regularities of the chronobiological changes in the samples are discussed.

The experiments were carried out with the support of the SPbU Resource Centers for (i) Physical Methods of Surface Investigation (ii) Diagnostics of Functional Materials for Medicine, Pharmacology and Nanoelectronics and (iii) X-ray diffraction studies. This work is supported by RFBR grant 19-02-00891.

Keywords: bone tissue, hierarchcal matter, chronobiology, electronic and atomic structure, biomedical applications, age effects, osteoarthritis.

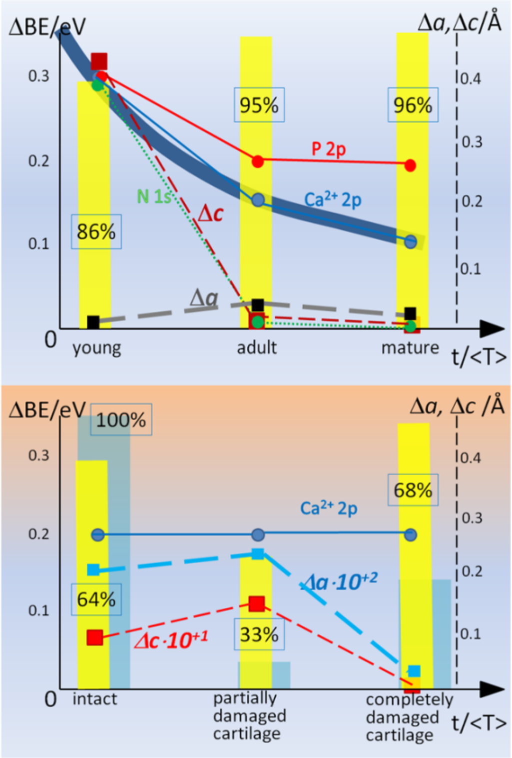

Figure 1. The fundamental chronobiological changes in nanostructure of cortex in young, adult and mature rats (upper) and femoral bone in OA knee compartment. The left and right scales correspond to the changes in electron BEs and lattice constants, respectively.

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Antibacterial nanostructured coatings on high-touch surfaces to prevent pathogen transmission in hospital settings.

M. Stanzione[1], G. G. Buonocore[1*], M. Lavorgna[1], A.M. Marcelloni[2], I. Amori[2], A.R. Proietto[2], A. Chiominto[2], E. Paba[2], A. Mansi[2]

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[2] INAIL (Italian Workers' Compensation Authority), Department of Occupational and Environmental Medicine, Epidemiology and Hygiene, Rome

Abstract:

Recently worldwide, a major challenge is represented by the prevention of Health care associated infections (HCAI). Environmental screening confirms that pathogenic microorganisms can persist for a long time, contaminating items, equipment and "common" area in hospital bed spaces and rooms causing serious infections and epidemic outbreaks[1]. To mitigate public health risk, besides hand hygiene, the main strategies include individual protection equipment (DPI), such as gloves, gowns, masks, as well as disinfectants' usage and high Touch Surfaces (HTS)' cleaning which could be regarded as a critical vehicles for bacteria via hands[2]. These methods appear ineffective to inhibit or to stop bacterial growth and often toxic solvents and/or detergents use may lead to environmental consequences, as well as increasing the risk of the onset of resistances. This evidence justifies the increased interest in the identification of new approaches based on antimicrobial coatings on sanitary surfaces[3], likely made of nanomaterials, both to ensure the heathcare safety and to reduce microbiological contamination. Different chemicals and technologies are presented on the market, but their applicability appears limited and their effectiveness in the hospital settings does not achieve conclusive results.

The objectives of this study are: i) development and characterization of new antimicrobial nanostructured removable polymeric coatings (AMC) of healthcare setting surfaces; ii) evaluation of in vitro efficacy of the innovative AMC by the ISO 22196:2011 and comparison of the results obtained by the identification of a new protocol, able to evaluate the reduction of bacteria contamination in more realistic conditions.

In details, our work comprises the following phases: - surface characterization of the developed PCL-based AMC of PP substrates (Figure 1) - *in vitro* evaluation of the antimicrobial efficacy of the developed AMC against bacterial strains well-characterized *S. aureus (ATCC 6538P)*, *E. coli (ATCC 8739)* and others responsible of HCAI.

It has been proven that this method proposes temperature and humidity conditions comparable to those of healthcare environments and provides more precise indications on the performance of the material in the target environment. Furthermore, results show that a rapid bactericidal action is certainly a not negligible aspect for the correct identification of the AMC to be used as a collective protection measure from infectious agents carried by objects or hands of patients and Health personnel.

Keywords: antimicrobial polymeric nanomaterials, patogen transmission, hospital acquired infections.

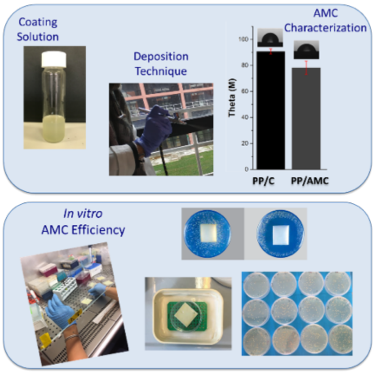

Figure 1: Coating preparation steps: coating solution and surface analysis, deposition technique, antimicrobial tests.

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Flexible NO2-Functionalized N-Heterocyclic Carbene Monolayers on Au (111) Surface

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[2] The Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Jerusalem, Israel
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Abstract:

The formation of flexible self-assembled monolayers (SAMs) in which an external trigger modifies the geometry of surface-anchored molecules is essential for the development of functional materials with tunable properties. In this work, it is demonstrated that NO2-functionalized N-heterocyclic carbene molecules (NHCs), which were anchored on Au (111) surface, change their orientation from tilted into flat-lying position following trigger-induced reduction of their nitro groups. DFT calculations identified that the energetic driving force for reorientation was the lower steric hindrance and stronger interactions between the chemically reduced NHCs and the Au surface. The trigger-induced changes in the NHCs′ anchoring geometry and chemical functionality modified the work function and the hydrophobicity of the NHC-decorated Au surface, demonstrating the impact of a chemically tunable NHC-based SAM on the properties of the metal surface.

Keywords: N-heterocyclic carbenes (NHCs), Self-assembly, Monolayers, Surface chemistry, NEXAFS spectroscopy.

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F. D. Toste, E. Gross et al.
Flexible NO$_2$-Functionalized N-Heterocyclic Carbene Monolayers on Au(111) Surface
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Figure 1: Flexible monolayers of NO$_2$-functionalized N-heterocyclic carbene molecules were assembled on Au surfaces. The reorientation of the surface-anchored molecules from tilted into flat-lying position was triggered by exposure of the sample to reducing conditions that facilitated reduction of the chemically active nitro groups.

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Interaction of bacteriophage lambda with lipid Langmuir Monolayers

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Abstract:

The specific and sensitive detection of pathogenic microorganisms remains a current scientific challenge and a practical problem of enormous significant. New advances in diagnostic and sensing technologies that can serve as alerts for bacterial contamination of food and water, enable highly selective and sensitive microorganism detection. Understanding the adsorption behavior of microorganisms on thin monolayers can provide a generic approach for the construction of the bacterial sensors. One of the current bacterial microorganisms' detections is based on culturing the microorganisms on agar plates followed by standard biochemical identification, which takes hours. Another bacterial detection approach is based on different kinds of biosensors, which in case of polymeric imprints change the shape of the microorganisms and results in its lack of detection. Due to the mentioned limitations, we suggest a different approach that takes into account a natural bacterial environment, such aqueous medium and the detection operation is harmless for microorganisms.

Our study aims at developing a technology for sensing microorganisms based on Langmuir-Blodgett technique. We suppose that the detection of the microorganisms is achieved by electrostatic interactions between the flexible amphiphilic layer and charged nucleocapsids. By using the Langmuir technique, we can measure the adsorption of nucleocapsids at the lipid monolayer at different concentrations and buffer conditions. By using cryo-transmission electron microscopy (cryo-TEM) we characterized the adsorbed structures at the interface. Further the obtained Langmuir film was transferred to solid surfaces and characterized by atomic force microscopy (AFM) and polarization modulation infrared reflection absorption spectroscopy (PM-IRRAS).

The research approach relies on the development and characterization of various Langmuir layers and their interactions with microorganisms.

Keywords: langmuir monolayer, bacteriophage lambda, air-water interface, lipid, biosorption, cryo-TEM

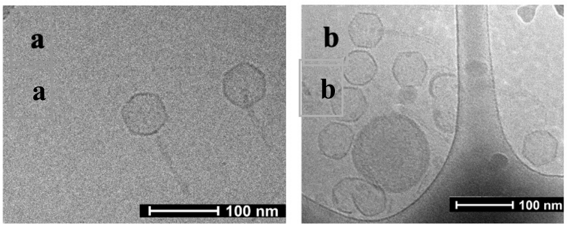

Figure 1: Cryo-TEM images of bacteriophage lambda in PBS buffer. Phage lambda from PBS solution (A) and from Langmuir Blodgett trough.

Integrated approach for exposure and health effects monitoring of engineered nanomaterials in workplaces and urban areas

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Abstract:
The aim of the present work, in the framework of the LIFE project NanoExplore, is to develop and demonstrate the feasibility of an integrated approach to conduct biomonitoring studies, characterize exposure levels and elucidate possible health effects deriving from exposure to engineered nanomaterials (ENM) in indoor workplaces and urban areas. This approach addresses current environmental, health, and safety questions about ENMs, by considering the integration of human biomonitoring studies with measured data on particle number concentrations (PNC), mass and particle size distributions (PSD) in the particle breathing zone (PBZ) as an instrument for developing consistent risk management guidelines for use by stakeholders from government, industry, NGOs, or the general public. To this aim, the definition and validation of a panel of candidate biomarkers of nanomaterial exposure and effects via inhalation has been conducted and biomonitoring studies to specify possible health effects were planned. In parallel the design of a wireless sensor network of 20 unattended, low-cost, portable and battery-powered devices that cooperatively monitor the concentration of ENMs and relevant physical environmental conditions in indoor workplaces and urban areas has been implemented. A risk analysis of possible effects on human health deriving from exposure to ENMs will be carried out in 5 case studies and the refinement of currently available Recommended Exposure Limits (REL) for metal oxides and low soluble carbon based materials will be achieved. In the long-term, the main goal of this study is to reduce potential adverse effects derived from the exposure to ENMs by setting up a harmonized health surveillance system, and promote new EU polices for the safe use of ENMs.

Keywords: ENMs, nanomaterials, biomonitoring studies, biomarkers, risk analysis, health effects, wireless sensor network, exposure levels.

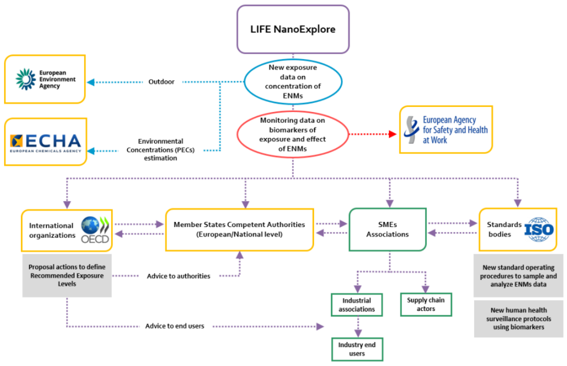

Figure 1: Figure depicting the impact of the project results and the interrelationships between the target audience, stakeholders and the project.

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

Functionalized porous materials for the detection of low concentrated metabolites and drugs

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Abstract:

The detection of low-concentrated biomolecules is a key issue in many areas of life sciences such as drug intoxication, medical diagnostic assistance, prevention of pathology's appearance and environmental integrity monitoring. Currently, in case of biological matrices, the main analytical methods used are either immunological or chromatographic. These two technics are powerful from both qualitative and quantitative point of view. However, some points limit their routine use for preventive superposes. Chromatographic methods require high qualified personnel, equipment and their maintenance are expensive and pre-treatment phases are time-consuming. Immunological methods are rapid, sensitive but have some limitations such as problem of interferences with other molecules or the impossibility of detecting certain biomolecules or drugs. The introduction of a solid/liquid interface to promote a controlled adsorption phenomenon can lead to the development of a complementary method for the detection of molecules at low concentration. Adsorption has the advantage of simultaneously allowing an overconcentration and a specific (or selective) interaction with a targeted molecule for routine uses with an acceptable costs and accuracy. In this presentation, two examples will be developed to illustrate the use of porous materials to detect, after adsorption, low concentrated biomolecules.

In the first example, the surface of a porous silica material was functionalized with specific functions able to realize "lock/key" type interaction with the target. Using an innovative synthesis procedure, hybrid mesoporous silicas with uniformly and densely covered polypeptides (glutathione) functions on its surface were prepared starting from a diblock copolymer composed of a polylactide hydrophobic block and a polypeptides hydrophilic block. The reactivity and accessibility of the confined glutathione functions towards benzoquinone that is a main metabolite of benzene were studied from a thermodynamic point of view. Adsorption parameters, such as the affinity between benzoquinone and porous materials functionalized with polypeptides and maximal adsorption capacities, were obtained. The crosschecking with the results of calorimetric experiments led to the energetic aspect of the interaction. These thermodynamic parameters were found similar to those determined in solution for the same interaction.

In the second example, gold nanoparticles were immobilized in the pores of the silica material (Figure 1). The resulting porous nanocomposite was the used as a substrate to detect oxazepam, a benzodiazepine metabolite.

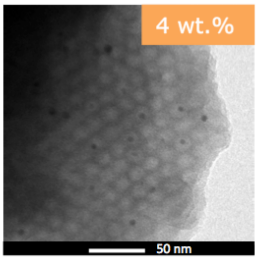

Figure 1: Transmission Electronic Microscopy picture of Au-based porous nanocomposite

This detection is based on the SERS effect that corresponds to a Raman signal enhancement observed when Raman-active molecules are adsorbed on "nanostructured" metal surfaces. The Raman response of oxazepam was coupled with its adsorption properties on such substrates allowing to understand the synergistic interplay between materials parameters/adsorption process and the drug detection threshold.

Keywords: porous silica, functionalization, detection, metabolites, drugs.

Towards a new generation of electrical biosensors based on 2D silicon nanowire networks for DNA and Thrombin detection

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Abstract

We present a new kind of Field Effect Transistors (FET) biosensors for DNA detection. They are based on 2D random networks of Si nanowires also called Si nanonets (Si NNs). Processing such biosensors relies on a simple implementation contrarily to more commonly studied 1D Si nanowires (NWs) based FET biosensors. 1D NW devices are obtained by top down lithography techniques, and their cost of fabrication and integration is a major hurdle towards their use for practical applications.

So far only used in our group, Si NNs exhibit many advantages: high surface-to-volume ratio, size providing an excellent environment to study a large number of biological entities, high fault tolerance and versatility in terms of materials on which they can be transferred.

Si NNs with controlled nanowire density are obtained from dispersion and filtration of bottom-up grown Si NWs. Following a transfer of Si NNs on a Si/Si_3N_4 substrate and a series of microfabrication processes, chips containing about 100 devices of Si NNFETs with various geometries are obtained (Fig. 1).

DNA grafting is carried out following a UV-assisted functionalization process using an epoxy-silane. This process provides the covalent grafting of DNA aptamer probes onto Si nanonets. AFM analyses corroborates that a correct biofunctionalization is achieved (Fig. 2). First results demonstrating electrical property changes of Si NNFETs upon DNA grafting will be presented emphasizing the key role of some experimental parameters (1).

Besides, implementing electrochemical biosensors for Thrombin detection is under investigation. In this case, Si nanonets are transferred on glassy carbon electrodes. Functionalization process relies on the generation of a poly(pyrrole)-NTA chelator film. Detection techniques such as cyclic voltammetry and electrochemical impedance spectroscopy are used.

This work emphasizes both the simple implementation and versality of Si NNs for various ways of electrical detection of different biomolecules opening the way for a new generation of electrical biosensors.

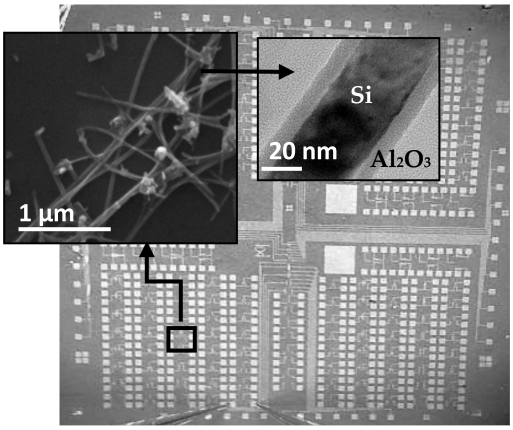

Figure 1 : Optical top view image of a chip (7x7 mm^2) containing different geometries of Si NN FETs. Insert (left) : SEM image of a Si NN connecting the metal electrodes after transfer on Si substrate covered with Si_3N_4, (right) : HRTEM image displaying an Al_2O_3 passivated Si nanowire.

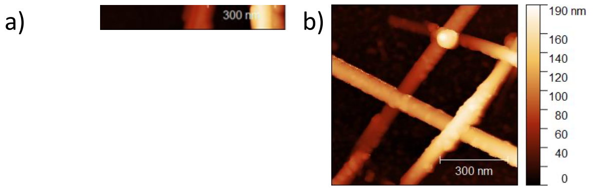

Figure 2 : AFM images of Si nanonet FET. a) Before biofunctionalization, b) After biofunctionalization and DNA hybridization.

Keywords: Si nanowire network, Si nanonet, field effect transistors, functionalization, DNA aptamer grafting

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Engineered Graphene decorated Aluminum-based plasmonic-nanostructures for biosensing applications in the optical Communication band

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Abstract:
The phenomenon of Surface Plasmon Resonance (SPR) has enabled real-time and label-free detection among bio-samples. A low cost and highly sensitive SPR based plasmonic sensor is the major requirement for the detection of any bio-analyte. In this work, for plasmonic activity initiation, Aluminum (Al) has been used as a plasmonic metal because of its low cost and wider spectral coverage[1]. To further increase the binding efficiency of the biomolecules with Al, a monolayer of Graphene (Gr) has been utilized due to its unique optoelectronic properties[2]. Al-based plasmonic nanostructures decorated with Gr layer, are engineered to demonstrate enhanced Sensitivity (S) and high Figure of Merit (FOM) for bio-sensing applications. The geometrical parameters for proposed structures are optimized using Rigorous Coupled Wave Analysis for the wavelength of 1550 nm in the optical communication band. The reflectivity curves with the variation in the refractive index of the analyte are captured to calculate the sensitivity and FOM for engineered plasmonic nanostructures as shown in Fig. 1. To demonstrate a bio-sensing application with the proposed design, the detection for the cancerous cells in liver tissues based on the change in their refractive indices is carried out. The proposed Gr decorated plasmonic nanostructure-based devices show the promising application in the optical communication band, employing Gr for functionalization purposes on Al-based periodic nanostructures.

Keywords: Aluminum, graphene, nanostructures, plasmonics, sensors, communication-band.

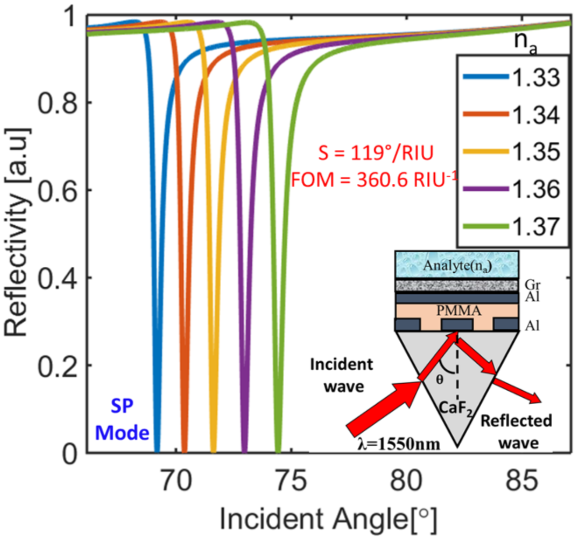

Figure 1(a): Reflectivity curves with the variation in the refractive index of analyte for proposed Al-based plasmonic nanostructures (schematically shown in the inset)

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Electro-Spun Silk-CNT Fibers to Stimulate Fibroblasts for Connective Tissue Repair

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Abstract:

Functional biopolymer scaffolds are in high demand for tissue regeneration. Among a variety of techniques to fabricate biomaterial scaffolds, electrospinning has gained considerable interest due to the simple process, low cost, high efficiency and the easy incorporation of additional components to make composite fibers. In our study, functionalized CNT was incorporated in collagen, spider silk or silkworm silk protein to generate biocomposite fibers by electrospinning. Comparative study was carried out to unravel the distinctive effect of CNT on collagen and silk fibers in fiber structure, mechanics, electrical conductivity, and in mediating fibroblast stimulation for tissue repair. It was found that the addition of a minute amount of CNT effectively improved protein fiber alignment and mechanical strength while retained high biocompatibility and decreased fiber diameter, mimicking native collagen fibers in the matrix of connective tissues. The addition of CNT also granted the fibers electrical conductivity to not only facilitate the electro-spun (E-spun) fiber formation but also mediate the electrical stimulation of fibroblasts from patients with chronic wounds or connective tissue disorder. We found that the silk-CNT fibers provided unique structural and mechanical cues to polarize and activate the fibroblasts producing collagen at a reduced collagen type I (COLI) to collagen type III (COLIII) ratio; due to the high conductivity, silk-CNT fibers effectively mediated the fibroblast stimulation to boost collagen productivity by more than 20 folds. The developed material and method offer a simple, direct and effective way to restore the function of patients' cells, which can be potentially used for personalized cell therapeutic treatment of diseases and health conditions associated with collagen disorder.

Keywords: silk protein, carbon nanotube, electrospinning, biocomposite fiber, fiber alignment, fiber mechanics, fibroblasts, electrical stimulation, tissue regeneration.

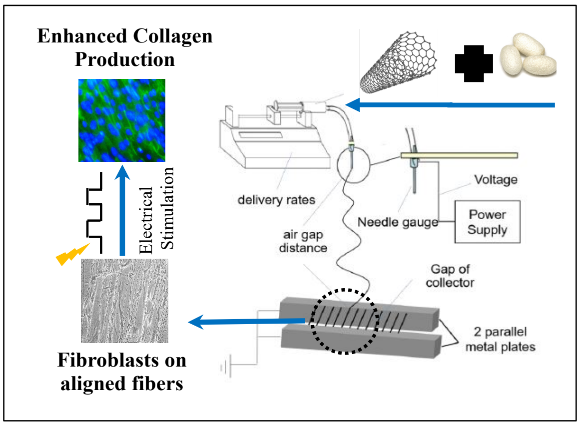

Figure 1: Silk-CNT composite fiber mediated stimulation of fibroblasts for enhanced collagen production. Aligned, mechanically strong and electrically conductive silk-CNT fibers were generated by electrospinning technique. Fibroblasts grown on the matrix were electrically stimulated to boost collagen productivity and reduce COLI/COLIII ratio, a favorable condition for connective tissue repair.

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Engineering Gold Nanoshells for Targeted Therapeutics & Point-of-Care Diagnostic Technologies

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Abstract:

Gold nanoshells are surface plasmon resonant (SPR) nanoparticles consisting of a nanoscale silica core surrounded by an ultra-thin gold shell.[1] Adjusting the ratio of the core diameter and the shell thickness tunes the absorption and scattering properties of the nanoshells throughout the visible and near-infrared (NIR) regions of the electromagnetic spectrum. This class of plasmonic nanoparticles has a wide variety of applications, including uses in optical filters, bio-sensing, and cancer therapy technologies. This presentation will introduce the interesting optical properties and color-engineering capabilities of gold nanoshells, detailing how their unique characteristics are harnessed to enhance their contributions to emerging technologies. Case studies will highlight their applications in the field of nanomedicine, specifically in designing lateral flow rapid diagnostic tests and developing photothermal therapies.

Lateral flow assays are easy to use, disposable diagnostic devices that test for biomarkers in samples such as saliva, blood, urine, and food. Billions of test strips are produced each year for the diagnosis of myriad diseases, ranging from those that are sexually transmitted or mosquito-borne to tuberculosis, hepatitis, and coronavirus, among others. Whereas 40 nm gold has historically been the classic nanoparticle choice for lateral flow assays, gold nanoshells can dramatically increase the sensitivity of lateral flow assays because each particle has 30× greater extinction (absorption plus scatter) than 40 nm gold (Fig. 1). Due to the dramatic increase in extinction, fewer binding events are required to observe a result at the assay's test line. This results in increased sensitivity and lower limits of detection to yield assays with enhanced performance at an affordable price.

Gold nanoshells are also of interest for photothermal therapeutics due to their biocompatibility and physical capability to efficiently convert light into heat. The NIR-absorbing gold nanoshells capture light that penetrates deep into biological tissues without being absorbed by the tissue and without damaging it. The heat generated is highly localized to the area around the nanoparticle, causing local destruction for targeted therapy with extraordinary spatial selectivity. Nanoparticle surfaces are readily functionalized for targeted association with biomolecules of interest and can even be engineered to target tumors and cancerous cells. In this way, nanoparticles serve as antennae to focus light and heat locally for targeted therapy. Examples of current clinical trials using this technology will be presented, including treatments for prostate cancer, hair removal, and acne therapy.

Keywords: gold nanoshells, surface plasmon resonance, plasmonic nanoparticles, lateral flow assay, point-of-care diagnostics, photothermal therapy, targeted therapeutics, nanomedicine.

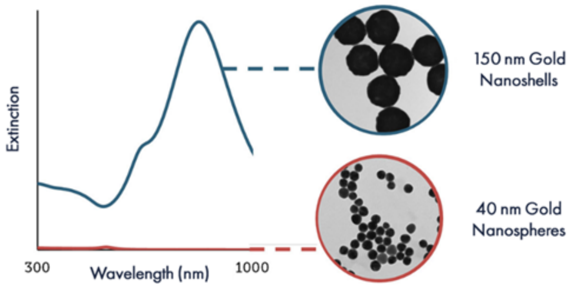

Figure 1: Gold nanoshells (150 nm) exhibit far greater extinction per particle than gold nanospheres (40 nm).

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NanoMatEn

Session III. A: Nanomaterials for Energy / Nanoelectronics

Nanowire solar cells: Challenging fundamental limits

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Abstract:
I will start to discuss the fundamentals of a nanowire solar cell with special emphasis towards the open-circuit voltage. It will be shown that the external photoluminescence efficiency is a major design criterium for enhancing the V_{oc}. The radiative limit for the V_{oc} is reached when the external radiative efficiency at the front side of the cell equals unity. I will discuss how to approach the radiative limit. Even at the radiative limit, the V_{oc} is still substantially decreased by a photon entropy loss due to the conversion of a parallel beam of photons from the sun into a randomized emission pattern, in which each individual photon is emitted into a random direction. The 46.7% ultimate solar cell limit for direct solar irradiation can only be approached, once the cell is capable to focus all emitted photoluminescence back to the sun. Our calculations show that 68% of the emitted photoluminescence at open-circuit is emitted into the HE_{11} guides optical mode that can be collimated back towards the sun. Assuming an internal radiative efficiency close to 100%, which is realistic for a GaAs solar cell, our calculations predict that it is possible to beat the radiative limit for the open-circuit voltage by 159 mV.

Nanophotonic engineering also allowed to reach a large short-circuit current (I_{sc}) by using tapered nanowires and forward Mie scattering for efficient absorption of the solar light into the nanowires, resulting in a 17.8% efficiency nanowire solar cell.

Keywords: Nanowire solar cells, fundamental limits, radiative limit, ultimate limit, entropy of light.

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Efficient oxygen evolution and gas bubble release achieved by a low-gas bubble-adhesion iron-nickel vanadate electrocatalyst

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Abstract:
Improving surface chemistry is a promising approach in addition to the rational alteration in the catalyst composition to advance water electrolysis. Here, we demonstrate an evident enhancement of oxygen evolution reaction (OER) on an iron-nickel vanadate catalyst synthesized by a facile successive ionic layer adsorption and reaction method. The vanadate-modified catalyst demonstrates a highly efficient oxygen evolution in 1 M KOH by requiring ultralow overpotentials of 274 and 310 mV for delivering large current densities of 100 and 400 mA cm^{-2}, respectively where vigorous gas bubble evolution occurs. Vanadate modification augments the OER activity from three aspects. (*i*) Both the electrochemical surface area (ECSA 47.1 cm^2) and intrinsic activity (318 mV to deliver 10 mA cm^{-2} per unit ECSA) of the catalytic sites are improved. (*ii*) The amorphous and roughened nanoparticle-comprised catalyst film exhibits a high surface wettability and a low-gas bubble-adhesion which is beneficial for the accelerated mass transport and gas bubble dissipation at large current densities. An *operando* dynamic specific resistance method is developed to study the gas bubble dissipation behavior where a significant decrease in the variation of the interfacial resistance during the OER is detected for the vanadate-modified catalyst. (*iii*) The introduced vanadate poly-oxo-anions with high charge density have electronic interplay with Fe and Ni catalytic centers. Raman study reveals the structural evolution of β-NiOOH and γ-FeOOH phases during the OER through the vanadate-active site synergistic interactions. Achievement of a high catalytic turnover of 0.12 s^{-1} put the developed iron-nickel vanadate among the best recent catalysts for water oxidation.

Keywords: oxygen evolution reaction, gas bubble detachment, iron-nickel vanadate, surface modification, water splitting.

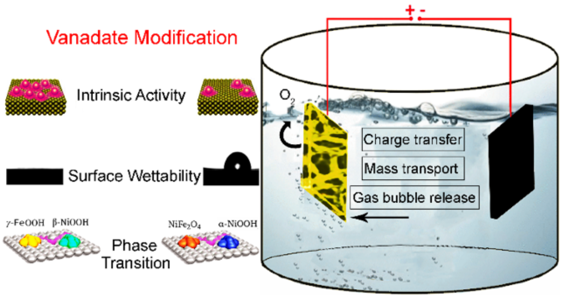

Figure 1: Figure illustrating anionic modification of FeNi catalyst with vanadate poly-oxo-anions boosting the intrinsic activity of Fe/Ni active sites, electronic active phase transformation, and gas bubble dissipation rate.

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Entrapped carbon quantum dots in a composite for oxygen reduction in anion exchange membrane fuel cells

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Abstract:

While the demand for renewable energy is growing, the development of materials that are sustainable and also to reduce the total cost in fuel cell applications is a major concern. Nowadays platinum is the catalyst most used in electrodes, bringing a huge onus to the mass production of green energy. In the process of achieving miles stones towards this problem, many catalytic materials were developed using metals (platinum, palladium), alloys (alloy1,alloy2), oxides (oxide1, oxide2), and metal-free catalyst [1]. One of the newest developments in the field of catalysts is the use of quantum dots.

Following this tendency, green quantum dots can be also used as a catalyst for the reduction of oxygen in fuel cells. In our laboratories, we started to study metal-free carbon quantum dots with both electron and proton-conducting as a catalyst in PEM fuel cells. We have chosen biocompatible carbon source materials such as glucose and citric acid [2] to synthesize carbon quantum dots and tuned their properties by using various functionalities introducing alkyl chains, different types of nitrogen, and preparing composites [3]. These quantum dots possess high stability and mixed conducting properties. The strategies followed to obtain Quantum Dots able to act as a catalyzer and at the same time reduce the costs of their production were hydrothermal, reduction followed by functional and composite with polymers. All materials obtained were chemically and electrically characterized by several techniques such as FTIR, NMR, SEM, TEM, CV, etc.

Keywords: electrocatalyst, biocompatible, mixed conductors, functionalization, nanomaterials.

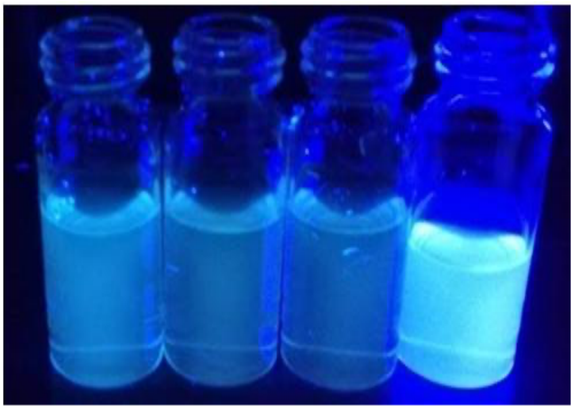

Figure 1: Carbon quantum dots under UV-lamp.

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Engineering of Electrode Materials and Interfaces in Perovskite Photovoltaics

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Abstract:

The perovskite solar cell (PSC) demonstrated remarkable solar conversion efficiency jumping from 3.8% to near 25% during the last decade The electron-selective layer (ESL) is a key component of the negative terminal of of PSC [1] The ESL should be pinhole-free, allowing fast electron injection and transport, and its conduction band minimum (CBM) must be properly aligned with the CBM of perovskite[2]. Amorphous ALD-made SnO_2 or TiO_2 films block holes for thicknesses down to several nm, but amorphous and crystalline ALD SnO_2 films differ in their conduction band positions. The energy of CBM is usually measured by optical spectra (giving the band gap) and photoelectron spectra (XPS, UPS) providing VBM. The electrochemical alternative is the flatband potential, which yields CBM, too. An electrochemical analysis of single crystal TiO_2 electrodes (anatase, rutile, brookite) together with vacuum and near-ambient pressure XPS and UPS studies as well as theoretical (DFT) modelling point at the effect of interface influencing the CBM positions [2]. Even 1-2 monolayers of water cause significant shifts. TiO_2 rutile thin films and or rutile/anatase double-layers turned out to be useful for PSC, too, outperforming even the anatase layers. Optically transparent rutile thin films can be most simply prepared by thermal oxidation of Ti at FTO [3]. A promising hole-conductor to replace spiro-OMeTAD is CuSCN, particularly if it is interfaced to reduced graphene oxide (rGO). The natural p-doping of CuSCN is demonstrated by both Hall-effect and by Mott-Schottky plots. The blocking function of CuSCN is tested by a newly designed redox-probe, $Ru(NH3)_6^{3+/2+}$. Raman spectra confirm that thiocyanate is the dominating structural motif over the isomeric isothiocyanate [4].

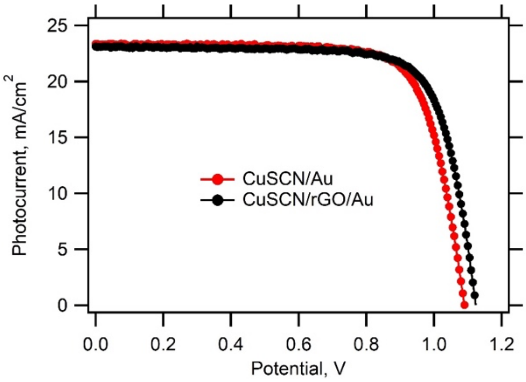

Figure 1: Photocurrent/voltage characteristics of a perovskite solar cell ($CsFAMAPbI_{3-x}Br_x$ perovskite) using CuSCN as a hole-conductor. The effect of a thin-film of reduced graphene oxide (rGO) interspersed between the hole conductor and the positive current terminal is shown [4].

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$CuCrO_2$ thin films out of stoichiometry as semi-transparent Hole Transparent Layer in performant and recyclable hybrid solar cells

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Abstract:

The improvement of the performances and photochemical stability of Organic Solar Cells (OSC) in atmospheric conditions, can be achieved by the replacement of chemical unstable and hygroscopic PEDOT:PSS[1] traditionally used as Hole Transport Layer (HTL) with p-type Transparent Conductive Oxides[2] (TCOs). In this work, $CuCrO_2$ thin films with various Cu/(Cu+Cr) cationic contents were synthesized by Aerosol Assisted Chemical Vapour Deposition to find a good compromise between transparency, conductivity, band alignment and devices performance. The resistivity, the transparency, and the energy gap are reduced increasing Cu/(Cu+Cr) ratio in the film. The composition of the $CuCrO_2$ film used as HTL was correlated to the performances of the solar cells. The strong chemical stability and mechanical resistance of the $CuCrO_2$ HTL allowed, through a simple chemical process, the recycling of the functionalized substrate composed of glass/ITO/$CuCrO_2$. This peculiar feature permitted the assembly of new solar cells over the same functionalized substrates, allowing the optimization of the Active Layer (AL). As highlighted results, we successfully substitute unstable PEDOT:PSS with $CuCrO_2$ out of stoichiometry able to enhance the performances of the devices. The greatest PCE in atmospheric conditions was achieved for Cu/(Cu+Cr) of 77% as the best trade-off between morphological, electrical and optical properties of the HTL, resulting in a PCE of 3.75% and a Fill Factor of 32% after the AL optimization. Moreover, the recyclability of the functionalized substrate will reduce manufacturing costs and processes, opening auspicious routes for prototyping and microelectronics.

Keywords: Transparent semiconductive oxides, TCOs, organic solar cells, oxides based HTL, recyclable pre-assembled substrates, sustanaible photovoltaic.

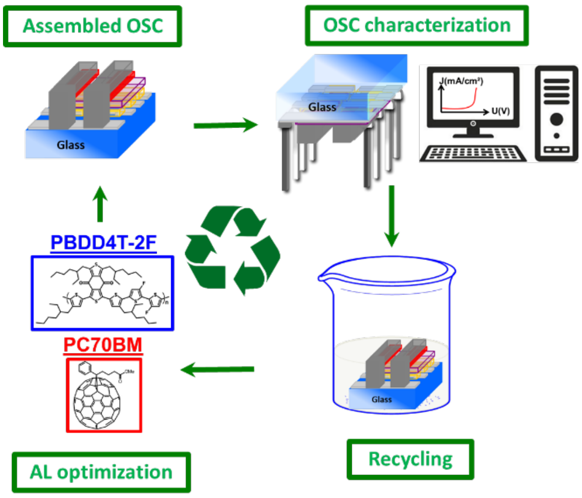

Figure 1: Figure illustrating the replacement of unstable PEDOT:PSS with $CuCrO_2$ out of stoichiometry. The chemical resistance of the oxides based HTL allowed the recycling of the solar cells, leading to the optimization of the active layer and the improvement the efficiency of the cells.

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Fluorescent and water-dispersible ternary alloyed Cu- and Al-co-doped ZnSeS/ZnS QDs

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Abstract:

Fluorescent and water-dispersible ternary alloyed Cu- and Al-co-doped ZnSeS/ZnS QDs with pure dopant emission have been synthesized through a simple aqueous synthetic route using 3-mercaptopropionic acid (3-MPA) as capping ligand (Figure 1). The influence of the Cu and Al-dopant concentrations has been systematically investigated in order to optimize the Cu-related photoluminescence (PL) emission. Through the increase of the dopants concentration, a significant increase of the PL quantum yield of Cu,Al:ZnSeS/ZnS QDs was observed (up to 30%). PL excitation and time-resolved PL measurements were also conducted to study the PL mechanism.

The crystal structure and shape of Cu,Al:ZnSeS/ZnS core/shell QDs were investigated using XRD, TEM and HR-TEM. XRD reveals that QDs exhibit the zinc blende crystal structure. With the increase of the Al dopant concentration, a slight shift of the XRD peaks to small diffraction angle corresponding to the incorporation of Al^{3+} ions in the ZnSeS host was observed. TEM and HR-TEM results show that the nanocrystals have a spherical shape and a size around 2.8 nm. The composition of the QDs was also confirmed by XPS measurements. In addition, Cu,Al:ZnSeS/ZnS QDs exhibit a high photostability.

Keywords: Quantum Dots, , Core/Shell, Photoluminescence, Co-Doping, Stability.

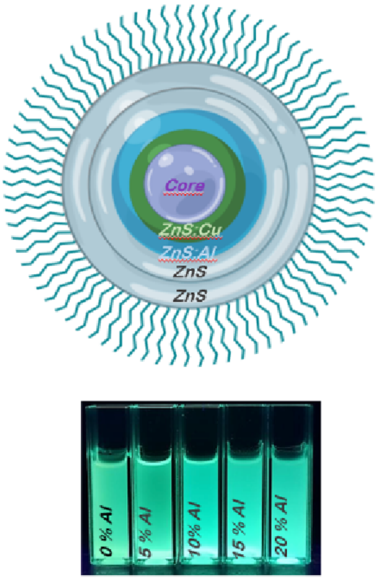

Figure 1: Schematic illustration of the structure of Cu,Al:ZnSeS/ZnS QDs and digital photograph taken under UV light illumination of the dots when varying the Al^{3+} dopant percentage.

References:

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High performance 2D micro-supercapacitor electrode composed of graphene with polydopamine as inserts

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Abstract:

Over the last years, graphene is deemed as one of the most promising electrode materials for EDLCs due to its large specific surface area (2600 $m^2 \cdot g^{-1}$), high theoretical specific capacitance (550 $F \cdot g^{-1}$) and high conductivity.[1] Among all the reported approaches to achieve a graphene-like material, the most favorable route is the reduction of GO and notably the electrochemical reduction of GO that is viewed as an economic, simple, fast and eco-friendly method with production possibility at a relatively large scale.[2,3] However, reduced graphene oxide (rGO) suffers from the small surface area due to the partial re-stacking of graphene sheets.[4] Therefore, it is necessary to develop an effective and feasible route to avoid rGO re-stacking to obtain graphene-based electrodes with a high specific capacitance and a good stability. Herein, we report graphene-polydopamine (PDA) composites as electrodes for micro-supercapacitor devices fabricated by a facile electrochemical approach.[5] We particularly address the rGO re-stacking issue by exploiting the PDA as a "chemical insert" between the graphene sheets but also explore the impact of PDA on the interfacial charge storage properties and the cycling performance. The optimized ERGO-PDA electrode possesses combined features of excellent capacitive behavior: high gravimetric and volumetric capacitances (178 $F \cdot g^{-1}$ and 297 $F \cdot cm^{-3}$, respectively, at 10 $mV \cdot s^{-1}$) with an excellent cycling stability (**Figure 1**). Additionally, the electrochemical quartz crystal microbalance analyses demonstrate a dominant cationic charge compensation and a very efficient interfacial transfer characteristics, since a totally reversible mass response during charge/discharge was observed for the optimized ERGO-PDA electrode. Here the favourable impact of PDA is shown to tackle rGO restacking issue, shedding light on the design of graphene based composite electrodes and can also be extended to other 2D materials for high performance electrochemical energy storage electrodes.

Keywords: EDLC, reduced graphene oxide, polydopamine, composite, microsupercapacitor.

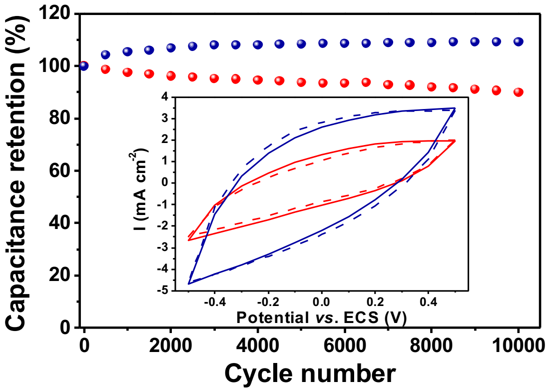

Figure 1: Capacitance retention of ERGO (red) and ERGO-PDA (blue) as a function of the number of cycles at 1 $V \cdot s^{-1}$, in 0.5 M Na_2SO_4.

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PEO-based porous silica hybrid materials as solid electrolytes for all-solid-state lithium ion batteries

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Abstract:
Dry polymer electrolytes based on poly (ethylene oxide), PEO, and Li-salt complexes are one of the cheapest, environmentally friendly and promising materials for developing safe, cheap and durable all-solid-state Li-ion batteries. Nevertheless, these rigid structures, that are interesting from the mechanical stability point of view, are characterized by a low ionic conductivity at ambient temperatures. In this context, the dispersion of oxide nanoparticles inside the PEO-matrix greatly improves the physicochemical properties of the complex due to the physical interaction between the oxide grains and the polymer matrix. Unfortunately, such a great effect drops at high loading-content, mostly above 10 wt%, owing to the particles agglomeration and the consequent Li-ion blocking effect.

In our work, we proposed a novel approach that leads to a porous composite electrolyte that consists in the use of a highe weight fraction of nanoporous silica than PEO polymer. Indeed, the polymer- salt complex is being entirely soaked inside the mesoporous silica matrix, offering the mechanical support for the electrolyte. Two different type of porous matrices were investigated : powders and thin films. They were functionalized with low molecular weight PEO polymer chains and with Li salt. Textural and structural properties of the starting materials and of the hybrid electrolytes were investigated. Furthermore, the electrochemical properties of the porous electrolytes will be discussed to demonstrate the feasibility of our materials as solid electrolytes in all-solid-state Li-ion battery cells.

Keywords: porous silica, functionalization, polymer, Li^+ ionic conductivity, Electrolyte

CNT and Graphene based Nanocomposite for Enhancing the Heat Transfer Processes in Hybrid Solar Panels

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Abstract:

The hybrid solar panels include both solar PV cells and a system of circulating cooling fluids for the optimal control of the operation temperature of the solar PV cells. The coupling of the two systems has to comply with different requirements and constrains. In order to address such challenges there were developed nanocomposite layers based on CNT and graphene mixtures

The proposed paper is synthetizing the results of the research project MULTISCALE – “Development of Advanced Materials by Integrating Nanomaterials and Nanotechnologies, Using Multiscale and Multiphysics Optimization, Dedicated to High-Performance Energy Systems” that is carried out in partnership between a University research group and industrial companies for innovative products and services. The grouping of industrial companies is including a manufacturer of high performance LASER systems and installation that have collaborated on the development and validation of a concept of biostimulation solutions of bacteria mixtures in anaerobic conditions using selected LASER beams.

The nanocomposite layers are engineered solutions of polymers using mixtures of CNT and graphene flakes as crosslinking and reinforcing agents but, also as fillers for obtaining the required properties of heat transfer, thermal expansion and mechanical properties.

Thre were tested several methods of processing the selected polymers and various types of ingredients.

The nanocomposite layers have been integrated in the architecture of the hybrid solar panels and tested in real conditions of operation.

The paper is synthesizing the research activities, the investigation methods and the experimental results obtained by the implementation of the project activities.

Keywords: CNT, graphene, nanocomposites, enhanced heat transfer.

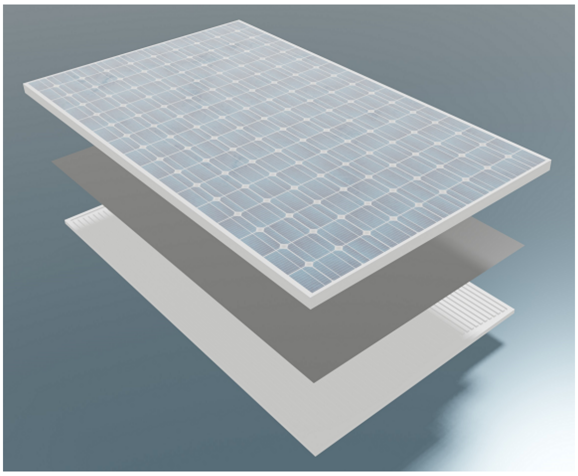

Figure 1: Architecture of the hybrid solar panel integrating the nanocomposite layer based on CNT and graphene mixtures.

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1D and 2D confinement in $CsPbBr_3$ perovskite nanocrystals

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Abstract:
We synthetized $CsPbBr_3$ nanocrystals showing confinement effects along one or two dimensions, called respectively nanoplatelets (NPLs) and nanosticks (NSTs) [1]. The joint analyses of TEM images and absorption and luminescence spectra collected at low temperature allow us to determine the anisotropy nanocrystals and their confinement effects. In NPLs of thickness L_z, the energies of observed transitions scale linearly as a function of L_z^{-2}, as expected in the strong confinement regime limit. A quasi perfect dependence is observed with decreasing L_z down to 4 MLs. In accordance with theoretical predictions [2], this result shows that, in these highly confined NPLs, the dielectric confinement effects (due to the dielectric contrast between the nanocrystal and its environment) do not play a significant role in the energy of the optical transition. The increase in the binding energy of the electron-hole pair which contributes to lowering the energy of the exciton transition is compensated by the increase in the carrier "self-energy".

At low-temperature, inhomogeneous broadening is the main contribution to the absorption linewidth. In highly confined NPLs, this inhomogeneous contribution definitely cannot result from the distribution in the NPLs thicknesses that would lead to huge displacements (≈ 100 meV). We believe that the lateral size dispersion is the origin of this residual broadening, in agreement with the small energy shifts of the exciton transition induced by the weak confinement in the lateral directions. NSTs show very good luminescence properties. We show the drastic dependence of the optical response with respect to the precise morphology of NSTs. They are very promising materials to study confinement and anisotropic shape effects on halide perovskite exciton properties, as lifetime, phonon coupling and fine structure.

Keywords: perovskite nanocrystals, 1D and 2D confinement effects, absorption and photoluminescence spectroscopy, TEM.

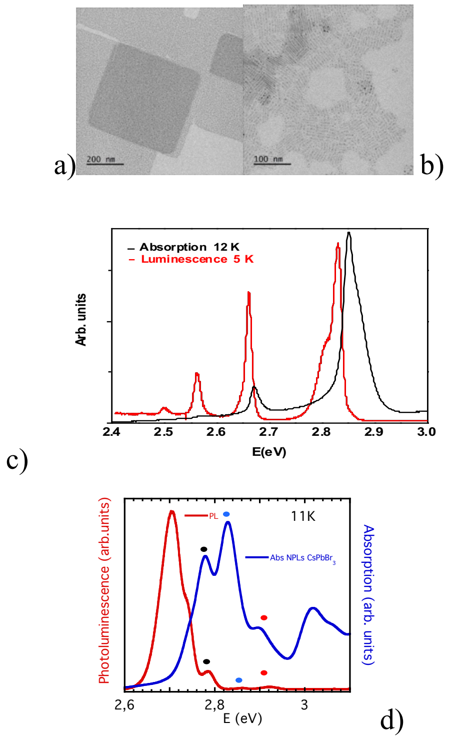

Figure 1: Transmission electron microscopy images of films of nanocrystals a) NPLs, b) NSTs. c) Absorption (black) and emission (red) spectra of NPLs at low temperatures. d) Absorption (blue) and emission (red) spectra obtained at T = 11 K in a film containing NSTs of average size 3nm x 4.5nm x 40nm. The colored dots identify the corresponding transitions in each of the spectra

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Fabrication of Polarized Emissive Optical Devices Based on Anisotropic Nanomaterials

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Abstract:

Nanomaterials play an ever increasing role in the development of novel optical devices. Such is the case in quantum-dot light-emitting diodes (QLEDs). In the case of nanomaterial-based display technologies, quantum-dots offer enhanced properties such as high quantum yields, tunable emission wavelength and a high color purity, attributed to their narrow emission spectra. Their implementation into optical devices, such as QLEDs, derives from their property to emit light, not only after kinetic excitement (photoluminescence), but also by injecting charge carriers in the form of electroluminescence. Electroluminescent quantum-dot LEDs are the main focus of several research fields with the aim of improving their optical properties. A typical system used for the optimization of these devices is CdSe/CdS.

The use of anisotropic nanomaterials, however, offer further advantages, which cannot be observed for 0-dimensional nanosystems, such as spherical CdSe/CdS nanoparticles. Indeed, anisotropic nanoparticles, such as CdSe/CdS quantum rods, exhibit polarized emission with high degrees of polarization (DOP) and high quantum yield. The energy-efficient generation of polarized light is of major interest for display applications. Aligned quantum rods have been reported as photoluminescent light sources for efficient LCD technologies, as well as active emissive layers in polarized emissive quantum-dot based LEDs (PEQLEDs).

For the use in macroscopic devices, large-area alignment of the quantum rods is indispensable to achieve strong polarization of the ensemble's emission. The following work offers insight into: (1) the optimized, reproducible synthesis of CdSe/CdS quantum rods by continuous flow processes, (2) the alignment of the quantum rods to produce films with high DOPs in ensemble and (3) the fabrication of optical devices such as PEQLEDs using the aligned quantum rod films.

Keywords: nanomaterials, LEDs, polarization, alignment, electroluminescence, optical devices, continuous flow, polarized emission.

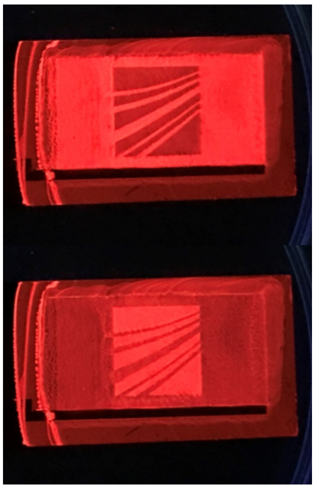

Figure 1: Quantum rod emission of an aligned film seen through a polarizer at two different angle orientations: 0° and 90°. The aligned films can be subsequently used for the fabrication of several polarized emissive optical devices.

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Gas sensors based on PbS colloidal quantum dots

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Abstract:

The detection of gas molecules such as NO_2, CH_4, CO and CO_2 is important in several areas, including environmental monitoring, building air quality, medical applications and industrial process control. This has stimulated a large demand for compact and reliable gas sensors. Among them, chemoresistive gas sensors based on semiconductor nanostructures proved to be quite effective due to their large sensitivity and simple device architecture [1].

Colloidal quantum dots (CQDs) are semiconductor nanoparticles suspended in solution phase that show strong quantum confinement effects, providing unique electrical and optical properties [2]. CQDs have attracted considerable attention for several electronic and optoelectronic devices, including field effect transistors, light emitting diodes, solar cells and photodetectors [3]. More recently, they proved to be promising building blocks for low-cost and high-performance gas sensors due to their large effective surface and versatile functionalization [4]. In addition, CQDs promote fast charge transfer providing superior gas-sensing characteristics with respect to their bulk counterpart and encouraging results have been published [5]. In this work we report on PbS CQD based sensors for room temperature gas detection.

Devices were fabricated dropcasting a solution of PbS CQD onto interdigitated metal contacts on silicon chips. A ligand-exchange procedure has been developed in order to tune the electrical conductivity and provide a satisfactory air stability. The sensor response has been measured for different molecules including NO_2, CH_4, CO and CO_2 and different concentrations in the 2.8-100 ppm range. A detection limit of about 10ppb has been estimated from the slope of the sensor response and its noise. The influence of the device thickness on the sensor response has been investigated and optimized. In addition, a sensing mechanism has been proposed.

Gas sensor based on PbS CQDs exhibited high sensitivity to NO_2, selectivity with some gas molecules, full recovery and good stability.

Figure 1 shows a typical sensor response to different NO_2 concentrations.

Keywords: colloidal quantum dot, gas sensors, lead sulphide, semiconductor nanoparticles.

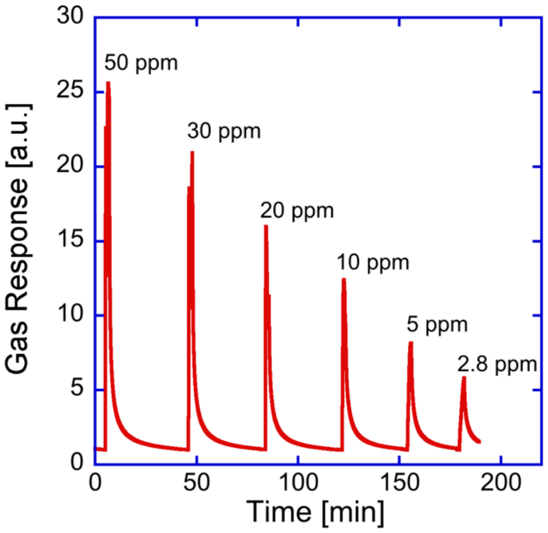

Figure 1: Response curves of the PbS-CQD sensor to different concentrations of NO_2.

References:

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Wavelength Selective Photodetectors based on PbS Colloidal Quantum Dots as Photoactive Layers and Optical Filters

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Abstract:

Wavelength selective photodetectors are of great interest in many applications such as light analysis, spectroscopy and imaging. Wavelength selectivity is typically obtained covering a photosensitive device with an optical filter with suitable absorption spectrum or with a series of dielectric materials specifically engineered to exploit optical interference and maximize transmission only in a short wavelength range. In both cases, the photodetectors and the optical filters are realized with different materials and their integration is not always straightforward. Here we propose a novel, wavelength selective, photoconductive device where both the photodetector and the optical filter are realized with the same material and can be easily deposited and integrated onto a variety of substrates. In particular, we employ PbS Colloidal Quantum Dots (CQD) and exploit their peculiar optical characteristics and the dependence of the optical absorption spectrum on the surface chemistry [1]. The photodetectors are realized by spin-casting the CQD solution onto interdigitated gold contacts and treating the as-fabricated film with a tetrabutylammonium iodide and methanol solution. This chemical treatment removes the organic ligands that cover the nanocrystals surface after synthesis and substitutes them with short I^- anions [2]. This process enhances the photoconductivity of the nanocrystal film and produces a slight modification of the absorption spectrum of the quantum dots. With the same CQD solution we also fabricate optical filters on glass without the ligand exchange process, thus avoiding any modification of the absorption spectrum. Finally, the glass filters are glued onto the photodetectors and responsivity characteristics vs. wavelength are measured. The final responsivity shows a strong wavelength selectivity; peak wavelength can be easily modified employing nanocrystals with different diameter and can be tuned between visible and near infrared.

Keywords: Wavelength-selective photodetector; Colloidal Quantum Dots photodetectors.

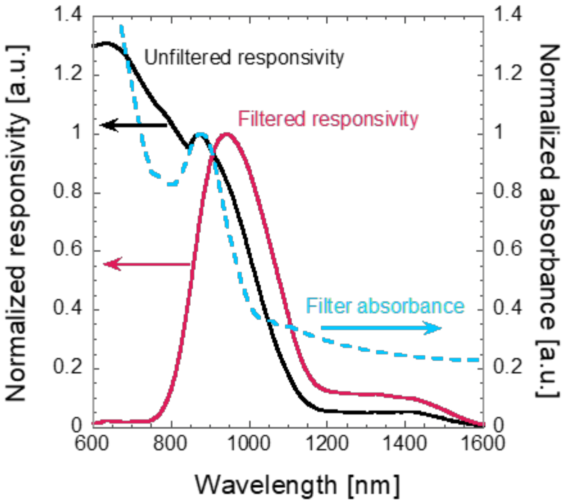

Figure 1: Normalized absorption spectrum of the PbS CQD optical filter on glass (cyan dashed line) and normalized responsivity of the unfiltered (black line) and filtered photodetector (red line)

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OLEDs on Flexible Substrates Nanostructured with UV-Nanoimprint Lithography

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Abstract:

Organic Light-Emitting Diodes (OLEDs) promise low-cost and large-scale roll-to-roll fabrication. The driving voltage can be easily decreased by doping the charge transport layers in so-called evaporated n-i-p OLEDs. However, fabricating n-i-p OLEDs by solution process is difficult. One easier way to reduce the driving voltage is to nanostructure the OLED interface. It leads to a local field distortion which enhances the carrier injection[1].

In this work, we show the influence of the nanopatterning on solution-processed OLEDs. The periodic nanogratings were made via UV-nanoimprint lithography, a low-cost and scalable process. A proprietary UV-resin "X166" from Stensborg A/S was deposited on a PET substrate. Using a transparent, flexible imprinting template, the structures were imprinted in the wet resin and exposed under UV light, forming the structured surface.The OLED stack was built on top of the nanostructured substrate by evaporating a silver layer and spin-coating the other layers. The UV-resin itself has no influence on the OLEDs properties as shown Figure 1. The fabricated nanostructured OLEDs exhibit a lower driving voltage than the planar OLEDs. It leads to an increase in luminous efficiency by a factor of 1.33. We also fabricated the nanogratings by a roll-to-roll process which has the main advantage to mold and cure the UV-resin almost instantanely. These nanogratings will be integrated in OLED device. The process we developed in this work allows to use any evaporated or solution-processed OLED materials on top of the gratings and it can be up-scalable to roll-to-roll fabrication for large surface devices such as OLEDs and organic photovoltaics.

The authors acknowledge support by Interreg (Project Rollflex, 1_11.12.2014).

Keywords: UV-nanoimprint lithography, periodic nanograting, roll-to-roll, OLEDs, solution-process, charge injection.

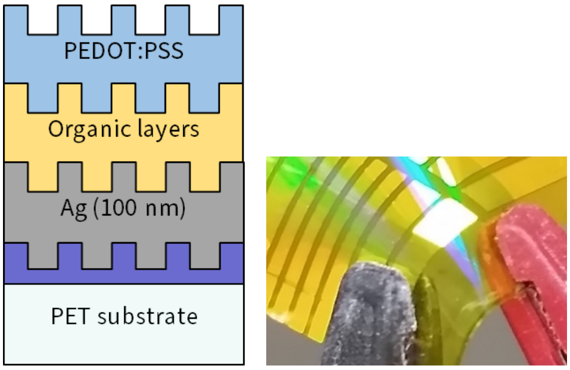

Figure 1: Nanostructured OLED stack (left) and picture of the flexible OLED under voltage (right).

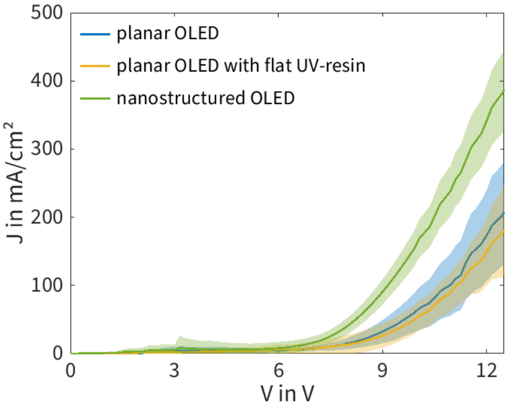

Figure 2: Averaged current density versus the applied voltage for different OLED devices: planar OLEDs, planar OLEDs with flat UV-resin and nanostructured OLEDs (nanostructured UV-resin).

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

Nanotechnology for Water Treatment

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Abstract:

Water is an essential element for life. However, with the growing world population and increasing demand for materials and resources, the availability of fresh water is diminishing at an alarming rate. Due to climate change and the excessive discharge of polluting substances in the natural aquatic environment, the United Nations (UN) estimates that by 2050, five billion people worldwide could suffer water shortages. The unacceptable reality is that currently, nearly 1 in 3 people (2.2 billion people) around the world still use sources of contaminated water, thus are exposed to waterborne diseases, which is causing about one million deaths annually. Finding affordable solutions to alleviate this pressing water crisis around the globe is one of the greatest challenges of this century.

Traditionally water and wastewater are treated using a variety of processes mainly based on separation and oxidation techniques such as activated carbon adsorption, reverse osmosis, membrane ultrafiltration, sand filtration, ion exchange, ozonation etc. However, these treatment processes, in addition to water pumping, consume a significant amount of energy, making the water industry one of the most energy-intensive sectors in the world. In the UK, for example, the water sector consumes 3% of the electricity the country produces and generates 1% of the carbon dioxide emissions. Current treatment technologies also suffer from degrading efficiencies as the infrastructure ages while they require chemicals to operate. Nanotechnology provides real opportunities to overcome these challenges through providing affordable and efficient water treatment technologies at industrial and household scales, thus benefiting industry and also communities without access to clean water.

This paper will report on experimental results from our lab on how nanotechnology has enhanced the performance of ozonation and membrane separation to remove contaminants from water and wastewater through the use of nanocatalysts and nanofillers. Ozonation in the presence of multiwalled carbon nanotubes (CNTs) was evaluated for the removal of a hazardous textile dye (methyl orange) under different operating conditions. The use of CNTs enhanced the dye removal rates by approximately 7 times more than conventional activated carbon (AC) relative to ozone alone. The study concludes that nanocatalytic ozonation with CNTs could be used as an effective wastewater treatment.

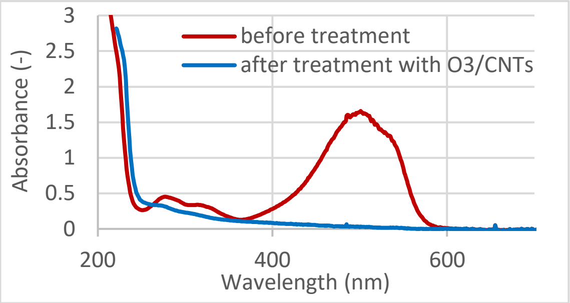

Figure 1: Effect of nanocatalytic ozonation on MO removal

In another study, we used a hydrothermal technique to synthesise a nanosize copper selenide visible-light photocatalyst to efficiently degrade estrone, an estrogenic hormone.

In separation processes, nanotechnology is also advantageous, and this is manifested in our study for the removal of endocrine disrupting compounds where nanosize polyamide was used to remove estrogenic endocrine disruptors estrone, 17β-estradiol and 17α-ethinylestradiol through a mechanism involving intermolecular hydrogen bonds with the -OH groups of the estrogens. The addition of nanofillers has also enhanced the performance of polyvinylidene fluoride (PVDF) membranes, prepared by the phase inversion technique from solutions containing CNTs. The content of CNTs was optimized and its incorporation in the membrane matrix was found to improve water permeability, improve rejection of contaminants and enhance the mechanical properties of the membranes. The study concluded that CNTs/PVDF membranes have a great potential to develop in a robust ultrafiltration membrane technique for water purification.

Keywords: Nanotechnology, water treatment, oxidation, separation, ozone, membranes, nanocatalyst, photocatalysis.

Nanocomposite Gels for Plugging of Fractures in Carbonate Oil Reservoirs

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[2] NORCE Norwegian Research Centre, Department of Energy, Stavanger, Norway

Abstract:

Excessive water production is a common challenge during water-flooding of oil reservoirs. The objective of the study was to identify and characterize nanocomposite gels for plugging of fractures in carbonate rocks. These gels were prepared of nanoclay and Enhanced Oil Recovery (EOR) polymers. Earlier a few studies have been conducted on nanocomposite gels for fracture plugging (Bai et al., 2018; Mohammadi et al. 2015), but most of them include Chromium (III) acetate or N,N'methylene-bisacrylamide as chemical crosslinkers.

The rheology and gelation time for bulk solutions were determined at 50°C by varying concentrations of nano-clay and EOR polymer, and brine composition. Interactions between carbonate rock and gelant and its effects on gelation was investigated by adding crushed rock to gelant solutions. Different types of glycols were evaluated for their potential to delay gelation. The most promising nano-clay and nanocomposite gels were further evaluation for their potential to plug fractured carbonate rock models.

Dispersion of the nano-clay was very sensitive to the brine composition. The nano-clay formed weak to highly viscous gels. The strongest gels were formed with hydrolyzed polyacrylamide and the weakest gels with the biopolymer Gellan-gum. Potassium and calcium were found to screen the electrostatic repulsion between nanoclay particles resulting in shorter aging time and stronger gels. Interactions of carbonate rock and gelant increased the calcium concentration in water and accelerated the gelation. Some of the glycols were found to retard the gelation reaction, but did not impair the strength of the gels. See example in Figure 1. Flooding in fractured carbonate rock models showed that both nanocomposite gels and nano-clay gels have potential to plug fractures in carbonate rocks. Nanocomposite gels were found to give higher resistance factor than nano-clay gels.

Nanocomposite gels gave excellent gel strengths and they can plug fractures in carbonate rocks and thereby reduce the water production during oil production. Further evaluations of nanocomposite gels should be carried out at higher temperatures and with other brine compositions. The gelation time can be delayed by adding retarders to the gelant solution, and this can allow longer transport of the gelant into target zones before formation of rigid gels.

Keywords: Nanocomposite, nanoclay, rheology, gelation time, gel strength, water production reduction, fractures, carbonate rock.

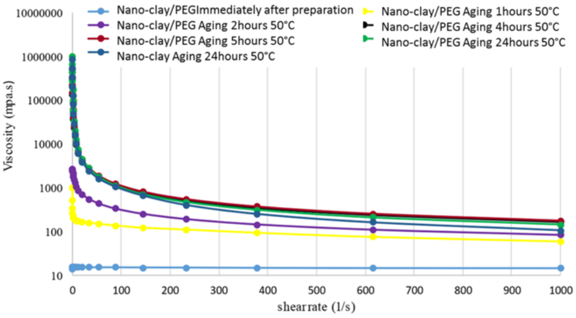

Figure 1: The viscosity of solutions of Nanoclay and retarder (PEG Poly Ethylene Glycol) and solution of Nanoclay was measured during aging at 50°C. The figure show that retarders can give low viscosity solutions at the injection point, and during aging very high viscous gels will be obtained, especially at low share rates. These gels were found to block fractures in carbonate rock models.

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Electroless Metallisation of Textiles using Copper-based Nanoparticle Catalysts for Inkjet Printing

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Abstract:
Maturolife (‘Metallisation of *t*extiles to make urban living for older people more independent fashionable’) is a three year, European Union (Horizon 2020) funded project aimed to develop assistive technology for older people incorporating E-Textiles.

Electroless copper plating is a technique where non-conductive materials can be metallised with copper after the substrate has been coated in a catalyst solution and it is a well-established technique for coating Printed Circuit Boards. Typically, the non-conductive surface is processed through pre-treatment to functionalise the non-conductive surfaces; then into a nanoparticle catalyst solution and finally into an electroless copper electrolyte containing a reducing agent, copper salt and a complexing agent. It results in a consistent conductive layer (µm scale) of copper.

In the electroless copper plating of textiles, various catalysts have been used including those based on Pd and Ag. However, these are relatively expensive and Pd is classified as a critical raw material. Previous work at Coventry University has established the feasibility of using Cu nanoparticles (CuNP) as an electroless plating catalyst[1,2] which offers advantages in terms of sustainability (Cu is earth abundant) and cost.

There are two approaches taken in this work to metallise textiles with electroless copper; bulk deposition (whereby the whole surface area is completely plated with copper) and selective metallisation (whereby copper plating occurs in a ‘pattern’). Selective metallisation allows for electronic circuits and sensors to be incorporated into textiles such as cotton, polyester and nylon. This brings electronic functionality to the textile enabling better electronic integration without losing comfort and flexibility. It also enables assistive technology to be ‘hidden’ reducing the stigma sometimes associated with the use of assistive technology in older people.

In this presentation, functionalised copper nanopowders and colloids were dispersed in a solvent and ultrasonicated at 20 kHz (80 W, 100% amplitude) for 30 minutes, to break down large clusters of particles. The dispersions were used as the catalyst for bulk plating and filled into ink cartridges for selective metallisation.

The copper nanoparticle catalysts were characterised by DLS, TEM, UV-vis Spectroscopy (556 nm) and XPS whilst the ‘bulk’ copper deposit was analysed using SEM, conductivity, adhesion, washing tests and deposition rate. It was found that copper nanoparticle (< 60 nm) catalysts resulted in electroless copper coating on the fibres of the textiles comparable to that found when a commercial palladium catalyst (<20 nm) was employed.

The most promising copper nanoparticle catalysts were then formulated so that they could be ink-jetted and successful copper patterning of the textile was achieved.

The authors would like to thank the European Union and the Horizon 2020 research and development programme for funding this work via Grant Agreement number: 760789**.**

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Application of multifunctional nanoparticles for cellulose fibers modifications.

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Abstract:

The increasing falsification of documents, clothing and packaging has serious economic and security implications for governments and companies, as well as for ordinary people and customers. Therefore, developing of a high-quality material protection strategy is an extrelmally important issue that needs to be addressed immediately. [1,2]

Here, we present a wide range of nanoparticles that may be used to modify of regenerated cellulose fibers in order to give them additional properties. Due to the addition of such modifiers, the fibers show superior properties, such as luminescence, upconversion, magnetism, or even a combination of these properties.[3–5] By controlling the size and quantity of the introduced nanoparticles, the mechanical properties of cellulose fibers, important from the the processing point of view, can be mantained. These fibers can be processed into fabric or paper that can be used to produce the final product (e.g. documents, cloths and labels).

The work was supported by a grant no. POWR.03.02.00-00-I026/16 co-financed by the European Union through the European Social Fund under the Operational Program Knowledge Education and the Polish National Science Centre (grant number 2016/21/B/ST5/00110).

Keywords: core/shell nanomaterials, documents and textiles protection, multifunctional nanoparticles, lanthanide(III) ions, luminescence & magnetism

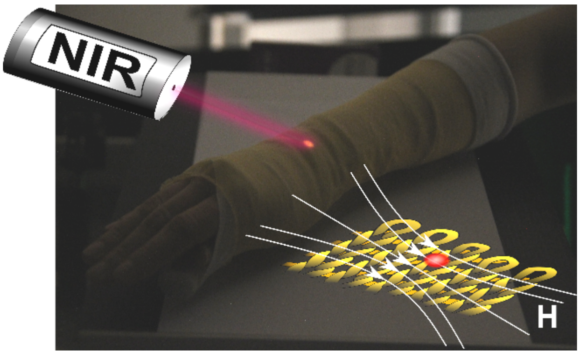

Figure 1: Photo illustrating a knitted fabric made of fibers modified with magnetic-upconverting NPs under the influence of NIR irradiation

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Nanotechnology for Water Treatment

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Abstract:

Water is an essential element for life. However, with the growing world population and increasing demand for materials and resources, the availability of fresh water is diminishing at an alarming rate. Due to climate change and the excessive discharge of polluting substances in the natural aquatic environment, the United Nations (UN) estimates that by 2050, five billion people worldwide could suffer water shortages. The unacceptable reality is that currently, nearly 1 in 3 people (2.2 billion people) around the world still use sources of contaminated water, thus are exposed to waterborne diseases, which is causing about one million deaths annually. Finding affordable solutions to alleviate this pressing water crisis around the globe is one of the greatest challenges of this century.

Traditionally water and wastewater are treated using a variety of processes mainly based on separation and oxidation techniques such as activated carbon adsorption, reverse osmosis, membrane ultrafiltration, sand filtration, ion exchange, ozonation etc. However, these treatment processes, in addition to water pumping, consume a significant amount of energy, making the water industry one of the most energy-intensive sectors in the world. In the UK, for example, the water sector consumes 3% of the electricity the country produces and generates 1% of the carbon dioxide emissions. Current treatment technologies also suffer from degrading efficiencies as the infrastructure ages while they require chemicals to operate. Nanotechnology provides real opportunities to overcome these challenges through providing affordable and efficient water treatment technologies at industrial and household scales, thus benefiting industry and also communities without access to clean water.

This paper will report on experimental results from our lab on how nanotechnology has enhanced the performance of ozonation and membrane separation to remove contaminants from water and wastewater through the use of nanocatalysts and nanofillers. Ozonation in the presence of multiwalled carbon nanotubes (CNTs) was evaluated for the removal of a hazardous textile dye (methyl orange) under different operating conditions. The use of CNTs enhanced the dye removal rates by approximately 7 times more than conventional activated carbon (AC) relative to ozone alone. The study concludes that nanocatalytic ozonation with CNTs could be used as an effective wastewater treatment.

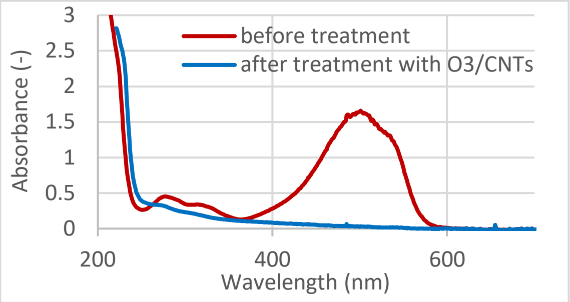

Figure 1: Effect of nanocatalytic ozonation on MO removal

In another study, we used a hydrothermal technique to synthesise a nanosize copper selenide visible-light photocatalyst to efficiently degrade estrone, an estrogenic hormone.

In separation processes, nanotechnology is also advantageous, and this is manifested in our study for the removal of endocrine disrupting compounds where nanosize polyamide was used to remove estrogenic endocrine disruptors estrone, 17β-estradiol and 17α-ethinylestradiol through a mechanism involving intermolecular hydrogen bonds with the -OH groups of the estrogens. The addition of nanofillers has also enhanced the performance of polyvinylidene fluoride (PVDF) membranes, prepared by the phase inversion technique from solutions containing CNTs. The content of CNTs was optimized and its incorporation in the membrane matrix was found to improve water permeability, improve rejection of contaminants and enhance the mechanical properties of the membranes. The study concluded that CNTs/PVDF membranes have a great potential to develop in a robust ultrafiltration membrane technique for water purification.

Keywords: Nanotechnology, water treatment, oxidation, separation, ozone, membranes, nanocatalyst, photocatalysis.

Quaternary Semiconductor Quantum Dots/Magnetic Iron Oxide Nanoparticles Covalently Coupled through Biopolymer Ligands as Multifunctional Nanohybrids: Insights of Photocatalytic Activity for Degradation of Water Pollutants

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Abstract:

Negligent discharging of industrial effluents and wastewater directly into water bodies pose a serious risk to the environment and human health, and therefore, it is an increasing global concern. Hence, innovative photocatalytic systems based on semiconductor nanomaterials have received special attention as a promising water treatment technology. Among several types of nanomaterials, ultra-small quaternary colloidal semiconductors (termed as quantum dots, QDs) such as Cu-In-Zn-S (ZCIS) and Ag-In-Zn-S (ZAIS) have demonstrated some advantages such as unique optical properties and low potential toxicity due to the absence of heavy metals (*e.g.,* Cd-, Pb-, Hg-chalcogenides) in their composition. Additionally, iron oxide nanoparticles have attracted remarkable research interest for environmental applications because they are magnetically responsive structures, which enable facile recovery and reuse. In this work, a novel multifunctional coupled nanostructure based on Cu-In-S/ZnS quantum dots (ZCIS QDs) and magnetite nanoparticles ($Co_xFe_{3-x}O_4$, MION) functionalized with carboxymethylcellulose (CMC) polysaccharide was designed and developed using a *"green"* aqueous colloidal synthesis. These hybrid nanoconjugates were extensively characterized, and the results demonstrated the effectiveness of CMC as a capping ligand for the direct production of both nanoparticles and the successful conjugation of ZCIS and MION through amide bonding using EDC as a *"zero-length"* linker. As an organic pollutant model, methylene blue (MB) was used to evaluate the photocatalytic activity of the ZCIS@MION coupled nanosystems under UV irradiation. The results showed the conjugation between the nanomaterials by the formation of covalent amide linkages (*via* R-COOH and $-NH_2$ groups), which demonstrated the capability as nano-photocatalyst in oxidizing MB as well as the influence of the QDs/pollutant ratio on the catalytic activity. Moreover, the nanostructures were recovery through a magnetic separation evidencing their potential to be reused in successive water treatment cycles. Thus, it can be envisioned that these novel hybrid coupled nanoassemblies based on non-toxic components and renewable biopolymer can be applied as advanced multifunctional nanoplatforms for eco-friendly treatment of polluted wastewater to avoid contamination and environmental pollution in water bodies and aquatic ecosystems.

Keywords: Wastewater treatment, Hybrid nanomaterials, Green synthesis of photocatalytic nanomaterials, Sustainable engineered nanostructures, Multifunctional nanophotocatalysts, Eco-friendly nanomaterials for water treatment.

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ZnO / Fe_xO_y for water depollution by photocatalysis under natural sunlight

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Abstract:

To solve pollution issues, photocatalytic infrastructures appeared rapidly as a sunstainble solution due to their ability to degrade and mineralize toxic organic pollutants into harmless compounds as H_2O, CO_2, NO_3^-. For this reason, we proposed to implement Zinc Oxide (ZnO) nanostructures onto civil engineering material surfaces, such as tiling and concrete, by low cost direct hydrothermal growth, in order to obtain photocatalytic paving blocks or photocatalytic motorway sound barriers[1]. Their good photocatalytic efficiencies under natural sunlight were already proved in our previous works[2].

To extend ZnO light absorption and improve photocatalytic efficiency, doping ZnO by adding iron (Fe) ions in growth solution was employed. Unfortunately, this method, for which the efficiency was already demonstrated, led to interactions between the non-conventional substrate and the dopant ions and to the decrease of the efficiency under natural sunlight for acid red 14 in water degradation (figure 1).

Thus, to challenge this impossibility, a post-grown ZnO/iron oxide (Fe_xO_y) cocatalyst synthesis method reducing the contact between substrate and doping solution was developed[3]. We therefore proposed a simple "drop, evaporation, calcination" method to strongly anchor Fe_xO_y on the surface of ZnO nanostructures grown onto silicon. Different deposition concentrations were studied. UV-Vis photospectrometry showed a widened absorption spectrum in visible range thanks to Fe_xO_y formation onto ZnO. Then, samples were used for the photocatalytic degradation of Methyl Orange in water, under natural sunlight (figure 1). Hence, the optimum sample was then selected and its iron leaching, lifetime and photocorrosion were also discussed in this work. Results demonstrated no iron leaching and promising lifetime. Nevertheless, nonhomogeneous iron oxide deposition seems to cause ZnO photocorrosion.

Keywords: Zinc Oxide, Iron oxide, Nanostructures, Cocatalyst, Photocatalysis, Water depollution.

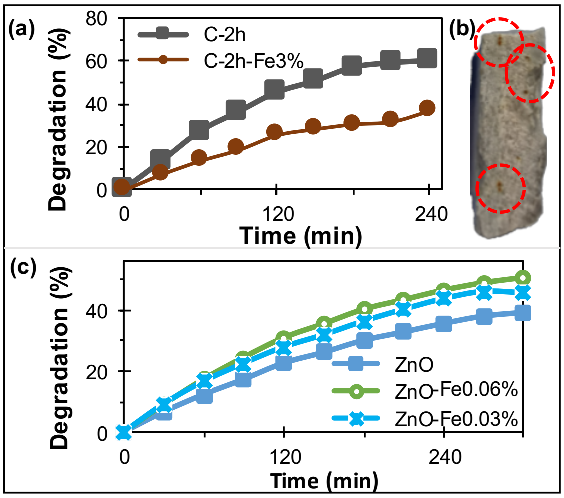

Figure 1: Figure illustrating problems (lower photocatalytic efficiency and interactions with iron), which were recorded with iron doping method in the ZnO growth solution, and solved by remplacing ZnO doping sample with the ZnO / Fe_xO_y cocatalyst sample to improve its photocatalytic activity without damage nor interaction with substrate during the ZnO modification process (c).

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Doped ZnAl-CO_3 layered double hydroxides as DeNO$_x$ photocatalysts with enhanced visible light harvesting

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Abstract:
Nitrogen oxides (NO$_x$, the sum of nitrogen monoxide, NO, and nitrogen dioxide, NO_2) are considered as one of the major air pollutants due to its several adverse and harmful effects. With the aim to confront this environmental problem, photocatalysis has been proposed as a viable technology to remedy NOx pollution (De-NO$_x$ action) at ppb-ppm levels in surrounding air [1]. Layered Double Hydroxides (LDH) are a group of materials with a structure similar to brucite ($Mg(OH)_2$). Due to its structural characteristics (uniform distribution of different metal cations, tunability and swelling properties) LDHs can be designed to use as photocatalyst to harvest different region of the solar spectra. Our previous work showed the efficiency of ZnAl-CO_3 LDH system to remove nitrogen oxides by photocatalytic oxidation [2]. In this study, the isomorphic substitution of Al^{3+} by Cr^{3+} or Fe^{3+} has been carried out to expand the light absorption to the visible region. The simple and ecofriendly coprecipitation method was used to synthetize nanoplatelets of ZnAlM-LDHs (M= Fe^{3+} or Cr^{3+}) with carbonate as the interlayer anion and different M/Al^{3+} ratios. XRD results showed that the crystallinity becomes poorer with the increase of Cr^{3+} and Fe^{3+}. ZnCr was successfully synthesized whereas the pure ZnAlFe was achieved with a ratio of $Fe^{3+}/Al^{3+} = 0.5$. The samples with higher chromium and iron content exhibited an increase in the BET area. The ZnAlM-LDH photocatalysts promoted the photochemical oxidation of NO molecules under UV–Vis irradiation (sunlight simulation), for which an increased NO conversion efficiency and outstanding De-NOx selectivity were found, in comparison to the undoped LDH. Furthemore, the doped LDHs exhibited an enhanced visible light absorption, which entailed an increase in the De-NOx performace under Visible light irradiation ($\lambda > 510$ nm). The enhancement in the photocatalytic results is related to the higher surface area of these samples and the better sunlight harvesting, as the iron/chromiun centres are responsible for the visible light catalysis. Moreover, the PL and EPR spin trapping measurements showed a decreased radiative recombination rate of the photocharges (Figure 1) and a favourable production of $\cdot O_2$- radicals in samples containing iron.

Keywords: LDH, Hydrotalcite, Photocatalyst, Nitrogen oxides, Visible-light.

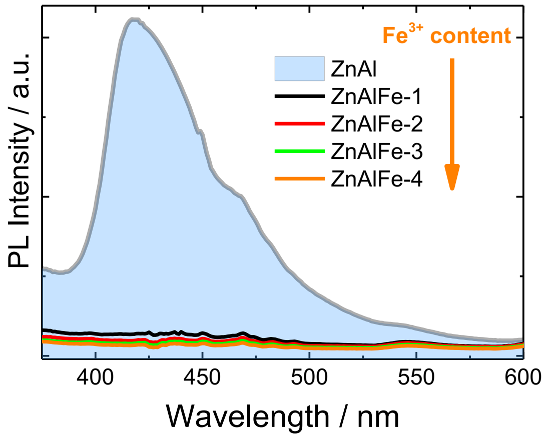

Figure 1: Photoluminescence (PL) spectra for the ZnAlFe-LDH samples ($\lambda_{ex} = 300$ nm).

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Transformation of CO_2/bicarbonates into formate over a Ni@Ni$(OH)_2$ nanocatalyst

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Abstract:

Conversion of CO_2 to chemicals is an attractive approach to decrease the content of this greenhouse gas in the atmosphere while providing chemicals from a waste. Conversion of CO_2 to formic acid or formate is particularly interesting as it is a valuable basic chemical and a liquid storage form of H_2.[1] Today, not a lot of heterogeneous catalysts are reported in the literature for this reaction[2] among which very few Ni-based systems.[3-5]

Taking benefit of the organometallic approach,[6] a foam-like, air-stable, Ni-containing nanomaterial was developed to catalyze CO_2/bicarbonate hydrogenation into formate. This nanomaterial was simply prepared by hydrogenation of the [Ni$(COD)_2$] complex in THF/EtOH without any stabilizer. It exhibited remarkable stability in air with an over two times higher catalytic activity than commercial Raney Ni catalyst in formate synthesis, at only 100°C, a significantly lower operation temperature compared to the 200-260°C previously reported. Deep characterization evidenced a core-shell structure with a surface layer predominantly composed of amorphous Ni$(OH)_2$ covering metallic Ni sites. The adsorption of bicarbonates on the catalyst proved to be a kinetically relevant step in the reaction. The Ni-Ni$(OH)_2$ interface appeared beneficial for the activation of CO_2 and H_2, thus leading to enhanced activities (Figure 1). This work reports a robust nickel-based nanomaterial that is a performant catalyst for CO_2 hydrogenation to formate in mild conditions. It also contributes to the understanding of 'structure-activity' relationship in CO_2 conversion.[7]

Keywords: CO_2; hydrogenation; formate; nickel; nanomaterial; catalysis

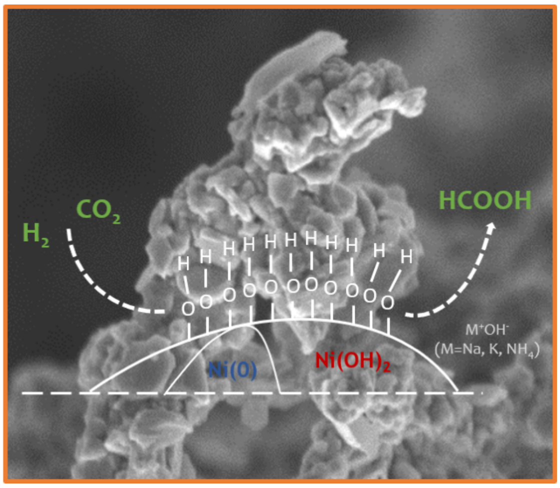

Figure 1: Schematic view of the transformation of CO_2 to formate over Ni@Ni$(OH)_2$ nanocatalyst

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Nanotech / Biotech
Session III. C: Nanotechnology for drug and gene delivery

The interplay of efficiency and biodegradation for inorganic nanohybrids in cancer or regenerative therapies.

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Abstract:

The emergence of multifunctional inorganic nanohybrids providing multiples functions recently paved the way to tailor-made therapeutic prescriptions and theranostic functionalities.

In cancer therapy, they have raised the prospect of thermal treatments that have few if any adverse effects. We recently compared the heating potential of magnetic nanoparticles under magnetic hyperthermia or photothermia[1,2], of plasmonic nanoparticles under photothermia[3], or the combination of both[4-8], towards synergistic solutions to complete cancer cell destruction. Different pre-clinical studies will be showcased, exploring in vivo these nanoparticles-based modalities. Among others, will be discussed - nanohybrids featuring a magnetic core and a copper sulfide shell to perform all at once magnetic hyperthermia, photothermal therapy and photodynamic therapy; - nanohybrids combining two plasmonic materials, to enhance the photo-thermal potential of each; - biosynthesized magnetosomes combined with a genetically encoded targeting unit in order to achieve enhanced photothermal treatment following intravenous injection.

The magnetism of iron oxide - based nanomaterials also provide cells with sufficient magnetization to manipulate them. Magnetic nanoparticles thus appear as a promising tool for tissue engineering opening up challenging perspectives. We developed magnetic-based methods to manipulate cells, towards the goal to provide magnetic artificial tissue replacements[9,10,11,12], that can be stimulated on demand, for instance to induce mechanically stem cells differentiation[13,14].

The therapeutic use of nanoparticles in cancer therapy or regenerative medicine application still raises the more general issue of intracellular nanoparticle long-term fate[15]. Cell spheroids models and magneto-thermal tools will be introduced, as tools to monitor long-term nanomaterials intracellular integrity. It evidenced a massive intracellular degradation[16], which could be prevented by a polymeric coating[17] or an inert gold shell[18,19]. Remarkably, human cells could also biosynthesize their own nanoparticles, from the intracellular degradation products of synthetic ones[20,21,22], with longer persistence, and limited toxicity.

Keywords: Magnetic and Plasmonic Nanoparticles, Biodegradation, Biocompatibility, Bioprocessing, Photothermia, Magnetic Hyperthermia, Tissue Engineering, Biophysical Cell Stimulations.

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Development of multifuntional MRI immunomodulating theranostic agents for Cancer

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Abstract:

The fight against cancer is a major challenge for public health. In this context, nanomedicine can help to fight more effectively against this disease via the vectorization of drugs. Nanotheranostics is a new field which combines the benefits of therapy and diagnosis using nanomaterials. Gadolinium is a contrast agent commonly used in magnetic resonance imaging (MRI). But as it is a toxic element so we must find some scientific solutions in order to reduce its toxicity and to make it biocompatible.

DOX is an anti-cancer drug widely used in chemotherapy however it has also side effects on healthy cells. The main goal of this study was to synthesize Au-Gd bimetallic nanoparticles in rods shape including the chemtherapeutic agent (DOX) for biomedical applications.

The chemotherapeutic agent grafting was done under two configurations, IN and ON. Physicochemical characterizations has shown that morphology and surface chemistry are different for these configurations. *In vitro* experiments indeed demonstrated that the configuration IN is better than the ON. More, relaxivity measures by MRI, has shown effectiveness of contras with these nanorods. This study demonstrated these nanoparticles can be suitable for diagnosis and therapy.

Keywords: Nanothernostic, MRI, bimetallic nanoparticles, gold nanorods, Gadolinium, Doxorubicin, biomedical applications.

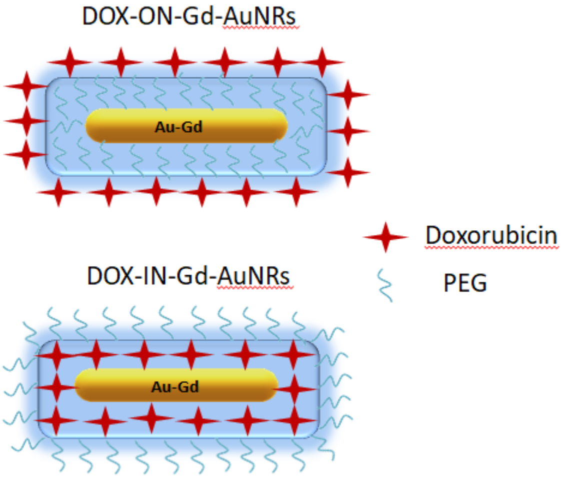

Figure 1: Figure illustrating the two methods of grafting therapetutic agent on bimettalic nanorods.

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Hybrid carbon nanotubes/gold nanostars for photothermal cancer treatment

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Abstract:

Cancer therapies are currently limited to surgery, radiation, and chemotherapy. These three modalities cause damage to normal tissues and lead to many undesired side effects. Nanotechnology offers impressive solutions in early detection, diagnosis, and personalized treatment of cancer and has the potential to generate novel and highly effective therapeutic agents. The unique physicochemical properties of carbon nanotubes (CNTs) make them good candidates for several applications in nanomedicine. Because of their tubular shape and mechanical flexibility, they have the ability to cross biological barriers and be internalized in cells [1]. Gold nanostructures are of growing interest in nanomedicine due to their large surface-enhanced Raman scattering activity, excellent photothermal properties, and low cytotoxicity. Both gold nanoparticles and CNTs show great photothermal properties and have been individually used as photothermal agents for thermal ablation of tumors under near-infrared light irradiation [2-3]. Photothermal therapy is based on the conversion of absorbed near-infrared light into heat and has been applied to kill malignant cells, while keeping the healthy ones safe. In this context, I will present the combination of multi-walled carbon nanotubes (MWCNTs) and gold nanostars (AuNSs) and the study of the potential synergistic effect of the conjugates for photothermal therapy. I investigated two strategies based on the decoration of MWCNTs with pre-formed AuNSs or the *in situ* growth of AuNSs on the nanotube surface. The conjugates were characterized by UV-Vis-NIR spectroscopy, transmission electron microscopy (TEM), and electron energy-loss spectroscopy (EELS; Figure 1). We expect that due to synergies, hybrid systems will be superior photothermal agents able to induce efficient cancer cell elimination.

Keywords: Carbon nanotubes – gold nanostars – cancer therapy – photothermal therapy.

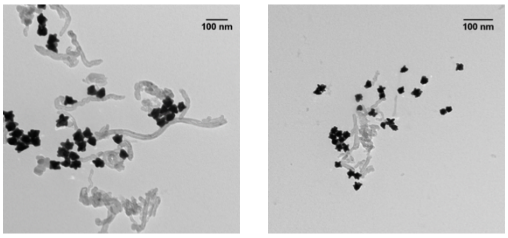

Figure 1: TEM images of CNT/AuNS nanohybrids.

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Design and Evaluation of Thermosensitive Liposomes Encapsulating Nedaplatin and Picoplatin with Controlled-Release and Enhanced Anticancer activity

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Abstract:

Thermosensitive liposomes (TSLs) are a promising triggered release delivery system used against solid tumors, with at least one formulation currently under phase III clinical trials [1], [2]. This paper presents data on thermosensitive liposomes loaded with nedaplatin (ND) and picoplatin (P), platinum-based anticancer drugs. The systems were characterized using different techniques. The entrapment efficiencies (EE%) and the in vitro release profiles were also investigated. The EE% was 74.19 ± 0.49 and 95.75 ± 0.49 for ND-TSL and P-TSL, respectively.

Additionally, the in vitro temperature-triggered drug release from the TSLs was demonstrated for all systems and showed good temperature control over the drug release (Figure 1 A & B). The preliminary investigation of these novel systems showed significantly in vitro anticancer activity combined with local hyperthermia against human mammary gland/breast adenocarcinoma cells (MDA-MB-231), as shown in Figure 1 (C, D, E, and F). Thus, our study suggests that TSLs could be considered a promising system for delivering platinum-based drugs to cancer cells. Hence, TSLs may contribute to reducing off-target toxicity in physiological conditions

Keywords: thermosensitive liposomes; triggered release; nedaplatin; picoplatin; breast cancer.

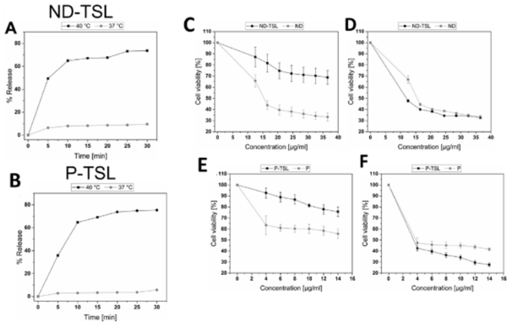

Figure 1: In vitro temperature-triggered drug release at 37 °C and 40 °C for (A) ND-TSL and (B) P-TSL.

Evaluation of the cytotoxicity of ND-TSL and free ND at different concentrations ranging from 12.5 to 36.5 µg/ml using MTT assay in MDA-MB-231 cells at (C) 37 °C and (D) 40 °C.

Evaluation of the cytotoxicity of P-TSL and free P at different concentrations ranging from 4 to 14 µg/ml using MTT assay in MDA-MB-231 cells at (E) 37 °C and (F) 40 °C.

An overall statistically significant decrease in cell viability was observed with drug-loaded TSL compared to free drugs.

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Isolation of extracellular vesicles from *Brassica oleracea* L. (Broccoli) and study of their effect on the metabolic activity of tumor cell lines

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Abstract:
After discovering the fact that plant-derived extracellular vesicles (PDEVs) can mediate interspecies communication, these natural derivatives are at the forefront of medicine and drug delivery. PDEVs offer multiple benefits in terms of size, low toxicity, good tissue specific targeting, excellent environmental safety and a significant potential for large scale production [1]. Considering their wide scale advantages, it can be expected PDEVs as next generation therapeutic drug delivery systems for the treatment of a wide range of diseases including cancers. In this *in vitro* study, we test our hypothesis that Broccoli derived extracellular vesicles (BDEVs), combining the antioxidant properties of their components (e.g Sulforaphane) and the advantages of their structure, can influence the metabolic activity of different cancer cell lines. BDEVs were isolated from homogenized fresh broccoli (*Brassica oleracea* L.) using a sucrose gradient ultracentrifugation method [2]. After ultracentrifugation, three bands of BDEVs were obtained (Band 1, Band 2 and Band 3) and their physical properties were assayed both by Dynamic Light Scattering (DLS) and Transmission electron microscopy (TEM). BDEVs mainly accumulated at the 8/30% (band 1) and 30/45% (band 2) interfaces of the sucrose gradient while a smaller band was also detected at the 45/60% interface (band 3) (Figure 1).
The average size measured by DLS was about 130 nm (band 1), 718 nm (band 2), and 553 nm (band 3). After determining their protein cargo (band 1 = 1692.5 µg/ml, band 2= 1201.4 µg/ml, band 3= 222.8 µg/ml), we tested the in vitro effect on the metabolic activity of different cancer cell lines (human colorectal adenocarcinoma cell line: Caco-2, human lung adenocarcinoma cell line: NCI-H441 and neuroblastoma: SHSY5Y cell lines), incubating them with seven doses of BDEVs (5, 11, 22, 45, 100, 500 and 5000 µg/ml). After 24h, MTT assay was performed to test the metabolic activity. In general, results showed that in presence of BDEVs the metabolic activity of different cancer cell lines was affected in a dose dependent manner compared with untreated cells. In this preliminary *in vitro* study, we have found that BDEVs can modify the metabolic activity of three different tumor cell lines and the level of modification varies differently depending on the cell lines and bands. Overall band 2 and 3 were found more toxic than band 1 irrespective of the cell lines. Our findings open to the possibility to find a novel “green” approach for cancer treatment, focused on using extracellular vesicles from natural substances.

Keywords: Plant-derived extracellular vesicles (PDEVs), Broccoli derived extracellular vesicles (BDEVs), tumor cell lines, DLS, TEM.

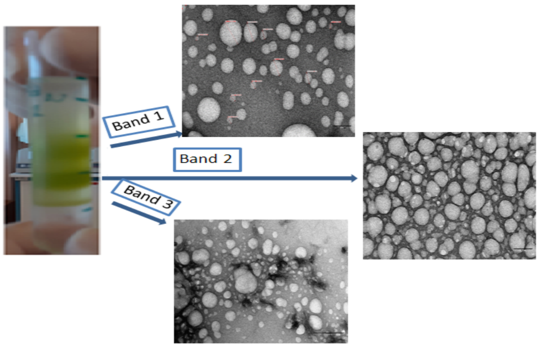

Figure 1: Figure illustrating the three Bands isolated from Broccoli along with their TEM observations.

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Evaluation of doxorubicin-loaded iron oxide nanoparticles synthesis and in vitro cytotoxicity on 4T1 tumorigenic epithelial cell lines

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Abstract:
Breast cancer is the most commonly diagnosed tumor formation in women around the world, which is also the leading cause of female cancer mortality [1]. Although significant progress has been made in the diagnosis and therapy of breast cancer, early detection of disease and antimetastatic treatment still remain a serious problem. The development of the next generation of cancer therapy modalities is relevant in modern oncology. Nanotechnology offers promising prospects in this direction [2]. Recently, the uptake of multifunctional iron oxide nanoparticles, combining both therapeutic and diagnostic capabilities, is gaining increasing attention in terms of cancer treatment, diagnosis, and targeted drug delivery [3]. This study is dedicated to the synthesis of Citric acid-modified Superparamagnetic Iron Oxide Nanoparticles (SPIONs) functionalized with an anti-cancer drug Doxorubicin (DOX), using controlled chemical co-precipitation method and study *in vitro* cytotoxicity of obtained magnetic nanofluids (containing Bare, Citric acid-coated, and DOX-loaded IONPs) on 4T1 tumorigenic epithelial cell lines (Figure 1). The synthesized samples were characterized using X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), Small-Angle X-ray Scattering (SAXS), Vibrating Sample Magnetometry (VSM), and UV-VIS spectrophotometry. To properly analyze and understand the behavior of 4T1 cancer cells after administrating Bare, Citric acid modified, and DOX-loaded IONPs in comparison with free DOX, a complex set of in vitro tests were used, including MTT assay, determination of the cell cycle, and IONPs uptake. Synthesized magnetic nanofluids containing Iron oxide nanoparticles (both Bare and modified with citric acid), revealed cytotoxicity on 4T1 cancer cells. However, the results showed the advantage of a combination of doxorubicin and magnetic nanoparticles. The DOX-loaded IONPs were more able to inhibit the growth and proliferation of 4T1 breast cancer cells *in vitro*, indicating that the system has the potential to act as an antitumor chemotherapeutic agent.

Keywords: SPIONs, tumor cells, Ferrofluids, Nanomedicine, magnetic nanoparticles, biomedical applications.

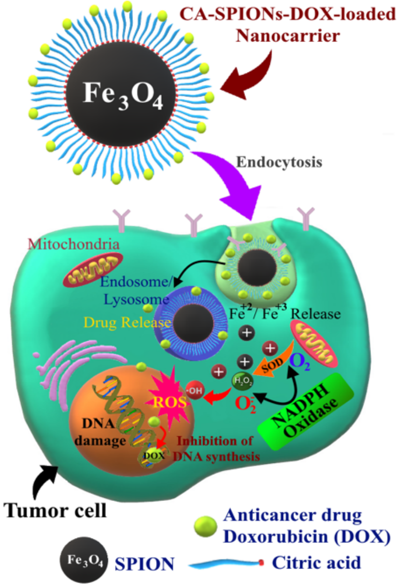

Figure 1: Schematic representation of the cytotoxic effect of iron oxide nanoparticles loaded with the anti-tumor drug doxorubicin.

Acknowledgements:
This work was supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG) under GENIE project (grant CARYS-19-976). The authors acknowledge the CERIC-ERIC Consortium for access to experimental facilities and financial support (Proposal number: 20177016).

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Magnetically-Driven Drug Release from Magnetosomes: Challenges and Applications

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Abstract:

Novel active release systems based on remote, non-invasive magnetic stimulus are a promise for therapeutic breakthroughs in nanomedicine. Magnetoliposomes and magnetosomes provide some appealing advantages, for instance large cargo capacities, stealth ability and lipidic formulations already approved for clinics. Also, targeted delivery enables new drugs with nonsuitable pharmacokinetics for clinical use to be implemented. Combining two or more of these capacities would represent a big step forward to increase biologically active molecules at the disease site. However, many challenges have kept these nanosystems from being already used in clinical trials, from chemical hurdles for an effective encapsulation of magnetic materials to the lack of reproducibility in the key parameters controlling the pharmacokinetic profile of the final product. We report on a novel nanosystem for remotely-controlled, magnetically-triggered magnetosomes, together with a recently developed instrumentation to measure the release profiles under magnetic field in real time.[1] We also discuss on the challenges related to repricibility of a) heating values of the magnetic nanoparticles, b) release profiles of the magnetosomes, and c) physicochemical parameters of the final formulation. As a complementary strategy we present a new approach using two complementary mechanisms to provide both site specificity and a triggering interaction for time and dose control.[2] The specificity is provided by a site-activated enzymatic disease marker (sphingomyelin) while the magnetic nanoheaters provide the time-controlled actuation mechanism to open the magnetoliposomal membrane. This concept has been tested through the sphingomyelin-containing magnetoliposomes labeled with the fluorophore indocyanine green, using the anticancer drug cisplatin. These engineered magnetoliposomes were characterized *in vitro* through leakage quantification and cell internalization studies. Our results showed a synergistic effect on the release of cis-Pt when both stress-related enzyme and magnetic field were applied to the carrier magnetoliposomes. In vivo studies using a squamous cell carcinoma tumor disease model showed similar synergistic effects, with a prolonged survival of the targeted delivery group versus free cisplatin.

Keywords: magnetoliposomes, stimuli responsive drug release; acid sphingomyelinase (ASMase); magnetic hyperthermia.

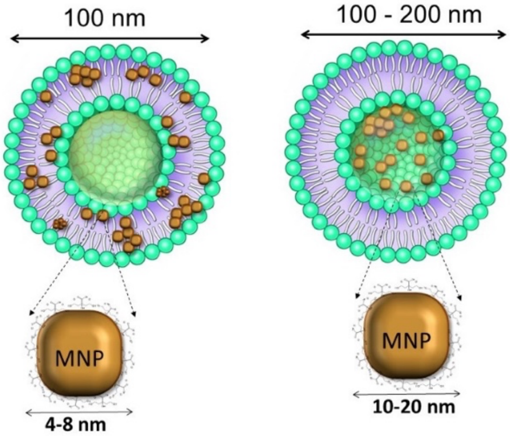

Figure 1: The two possible structures of the magnetoliposomes, depending on the synthesis protocol, and coating and average size of the magnetic nanoparticles (MNP). In both cases the aqueous cargo space contains the therapeutic cis-Pt drug to be released.

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Understanding of in vivo behavior of nanosystem based on magnetic nanoparticles

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Abstract:

Inorganic nanoparticles possess unique physical properties which give the possibility to call a respond to external stimuli (light, magnetic field, ultrasound, etc.) and to detect their accumulation in vivo (by MRI, optical tomography, etc.). These properties allow us to control accumulation of nanoparticles in target site to make a decision about the advisability of nanotherapy and to promote control drug release. However, the targeted delivery of nanoparticles remains a challenge. The research was aimed at studying of in vivo behavior of nanoscale systems, based on magnetic nanoparticles and designed for targeted diagnostics and / or therapy of malignant neoplasms.

Fluorescent-labeled, PEGylated iron oxide magnetic nanoparticles (MNPs) were synthesized and covalently conjugated with peptides: pH-low-insertion peptide (pHLIP) [1] or non-inserting counterpart pHLIP-K.

For investigation of the MNPs behavior in vivo two models of breast cancer tumor were established: 4T1 (in inbred BALB/c mice) and MDA-MB231 xenografts in NU/J mice. The blood, liver, spleen and tumor samples were collected in definite intervals after nanoparticles intravenous administration. Tissue samples were homogenized and stained for flow cytometry analysis using a set of antibodies. To dedicate the penetration mechanism of magnetic nanoparticles into the tumor intravital microscopy was implemented. To study the distribution of MNPs in the tumors, immunofluorescent analysis of tumor cryosections was performed. The whole set of obtained data showed that blood cells play very important role in penetration of magnetic nanoparticles into the tumor. The results provide valuable information about the nanoparticles behavior in vivo, and also allows us to propose approaches to improve the biodistribution of nanoparticles for biomedical application.

Keywords: magnetic nanoparticles, tumor, targeted delivery, peptide, tumor penetration, intratumoral biodistributon.

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Bioencapsulation capabilities of HepE Nanoparticles and their medical Applications

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Abstract:

A modularized theranostic capsule, Hepatitis E Virus Nanoparticle (HEVNP) modified with a surface cysteine for chemical conjugation, was chosen as a platform of modularized theranostic capsule because of its possibility of weakening the immunoresistance against the pre-existing HEV antibodies[1]. The engineered HEVNP after conjugation with LXY30, a ligand peptide with a high affinity for human malignant breast tumor cells, showed specific targeting to breast tumor cell both *in vitro* and in *vivo*, indicating that delivery route of HEVNP can be manipulated to facilitate targeted delivery of diagnostic or therapeutic reagent to pathologic foci. Besides conjugating the specific-cell targeting ligand on the surface, the utilization of modularized theranostic capsule can be expanded by using the interior space of HEVNP as well. A DNA vaccine was proposed using HEVNP encapsulating foreign DNA to stimulate mucosal and systemic immune response by oral administration. Conversely, the HEVNP sequence has been optimized to not encapsulate viral RNA, forming highly stable non-infectious capsids capable of reversible *in vitro* assembly through cation mediation. As an expansion of the HEV encapsulation research, negatively charged siRNA and gene editing machinery, such as Cas9/gRNA ribonucleoprotein (RNP), could be also encapsulated into the interior of HEVNPs, which provides broad possibilities for gene therapy. The HEVNP is also capable of encapsulation of magnetic nanoparticles such as ferrite, for both diagnosis under MRI and thermotherapy. It could also be applied to tumor-targeted-hyperthermia induced by radio frequency (RF) electromagnetic radiation using heat activated ferrite particles encapsulated in the tumor targeted theroanostic capsule[3]. Therefore, the successful tumor targeting and encapsulation capability of HEVNP could be used as modularized theranostic nano-capusule in various medical applications from oral vaccine, cancer diagnosis, tumor-directed hyperthermia treatment, organ/tissue targeting gene therapy, and other therapeutics lacking of targeting capability.

Keywords: bioencapsulation, theranostic capsule, nanoparticles, chemical conjugation, cancer targeting, gene therapy, gene editing, hyperermia, oral vaccine, DNA vaccine, MRI.

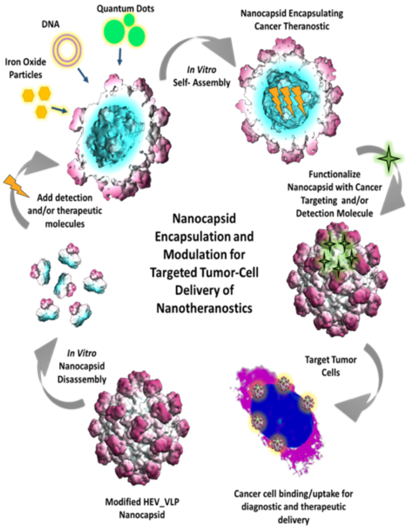

Figure 1: Figure illustrating the fundamental concept that HEVNP are proposed as targeted tumor, nanotheranostic delivery capsule by (i) surface conjugation of cancer targeting ligand; (ii) encapsulating different theranostic payloads, such as inorganic nanoparticles, nuclei acids, protein/peptide etc. to serve as modularized theranostic nano-capusule in various medical applications from oral vaccine, cancer diagnosis, tumor-directed hyperthermia treatment, organ/tissue targeting gene therapy, and other therapeutics lacking of targeting capability.

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Modified zinc oxide nanoparticles as potential drug carriers

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Abstract:

Nanotechnology has become an integral part of modern technologies. Pharmacology is one of many areas of using nanomaterials. Nanoparticles act as carriers of medicinal substances. The scientific literature reports that, despite many benefits of this type of drug delivery systems, nanocarriers can accumulate in healthy tissues and organs, as well as may have toxic effect on healthy cells [1].

The aim of the work was to develop innovative carriers of medicinal substances based on modified nanostructured zinc oxide, whose properties would allow for their safe use in living organisms. The less toxic nanocarriers have been prepared by attaching mannose to zinc oxide particles [2]. The presence of mannose reduces or eliminates the toxic properties of the entire product. Zinc oxide nanoparticles have been functionalized *in-situ* at the time of their production by incorporation monosaccharide molecules into their surface. The reduction of toxic properties should be seen as limiting the release of metal ions from nanoparticles under the effect of the attachment of surrounding particles (monosaccharides) to nanoZnO. These ions influence the formation of reactive oxygen species (ROS), which in turn trigger intracellular oxidative stress. Ion release limitation is tantamount to reducing the toxic properties of nanoparticles. Also nanoparticles captured by the cell may be dissolved inside, releasing metallic ions. It is predicted that the presence of monosaccharides on their surface will significantly reduce their penetration into the cells, as well as inhibit their dissolution. A series of zinc oxide nanoparticles modified with mannose has been obtained. All processes have been conducted in the field of microwave radiation. The products were differentiated depending on the values of the process parameters such as process time, process temperature, amounts of reagents, molar ratios of reagents, pH of the reaction mixture and sonication time (quantitative parameters). The sizie and electrokinetic potential of the products were characterized by DLS technique. The specific surface along with pores diameter and volume were analysed by BET technique. Also, XRD, FTIR studies have been performed. The surface was also assessed by SEM-EDS microscopy. It has been confirmed that the releasing of zinc ions from the modified products have been reduced comparing to the basic zinc oxide nanoparticles. The results of the study will permit us to discuss a new type of products which are dedicated to the pharmaceutical industry, in particular to producers of targeted drugs.

This work is a part of the project “A method of producing non-toxic carriers of active substances based on nanomaterials,” supported by the National Centre for Research and Development, Poland under the agreement LIDER/20/0080/L-9/17/NCBR/2018.

Keywords: nanotechnology, zinc functional materials, drug carriers, nanomaterials, transport systems.

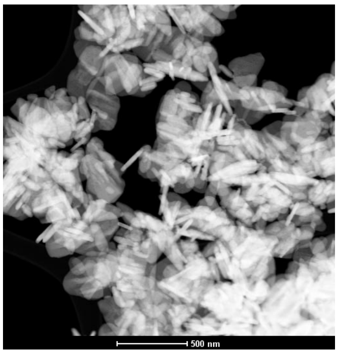

Figure 1: HR-TEM microphotography of zinc oxide nanoparticles modified with mannose.

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Nanotech / Biotech
Session III. D: Nanotechnology for life science

Pancreatic Cancer Treatment Using Magnetic Hyperthermia

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Abstract:

Pancreatic ductal adenocarcinoma (PDAC) is the most frequent type of pancreatic cancer, with a very poor prognosis and an average five-year-survival rate of 9 %. Therefore, there is an urgent need of new therapeutic strategies. These tumors are characterized by the deposit of a large amount of stroma, which prevents the diffusion of chemotherapeutic agents towards tumor cells and inhibits the response of the immune system. As a result, new therapeutic strategies are now focusing on the disruption of this stroma in PDAC.

In our group, we used nanotechnology, and in particular, magnetic hyperthermia (MH), to increase the permeability of the tumor stroma. Magnetic hyperthermia was proposed as a promising therapy for cancer treatment. Iron oxide nanoparticles are the most commonly used material for this purpose, given their biocompatibility and physical and chemical properties. Under exposure to an external alternating magnetic field (AMF), the local temperature near the magnetic nanoparticles (MNPs) increases and this phenomenon may be used to trigger cell death.

A 3D cell culture model using a pancreatic tumor cell line (MiaPaCa) was used for *in vitro* optimization of the AMF conditions. Then, the MH treatment was tested in a heterotopic xenograft mouse model using the optimal AMF conditions. MNP biodistribution, cell death and immune response triggered by MH were evaluated through different techniques: magnetic measurements, flow cytometry, confocal microscopy and histochemical staining. Our results evidence the important effect of the nanoparticle biodistribution after intratumoral injection in the treatment effectiveness.

Keywords: pancreatic cancer, magnetic nanoparticles, iron oxides, biodistribution

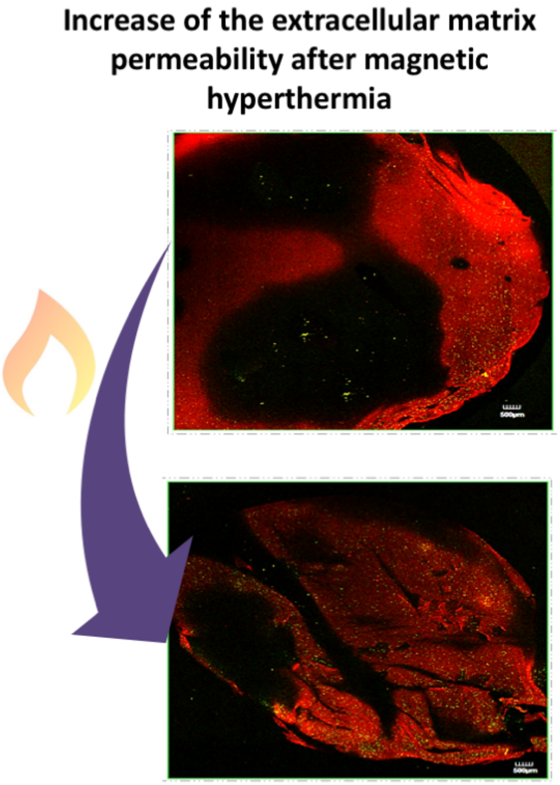

Figure 1: Map image of confocal microscopy of 3D cell culture without (up) and with (down) the alternating magnetic field exposure. The image shows the overlay of two channels: green fluorescence of the labeled cells and red fluorescence of the magnetic nanoparticles. Scale bar is 500 µm.

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Nanoemulsions stabilized by protein to encapsulate curcumin for a topical application.

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Abstract:

Curcumin has many possible applications in the pharmaceutical field through its anti-inflammatory, anti-oxidant, antimicrobial or anti-cancer properties [1]. Despite its proven usefulness in the therapeutic field, curcumin is a difficult molecule to formulate because of its low solubility and its degradation in aqueous media. To solve these major issues, the choice of innovative formulations seems to be essential. These hurdles could be overcome by encapsulating curcumin in nanoemulsions, knowing that this kind of system has been little explored with curcumin. Nanoemulsions (NEs) are characterized by very fine droplets with a mean diameter ≤ 200 nm and a narrow size distribution [2]. Nanosized droplets confer to NEs their kinetic stability to the gravitational separation, the flocculation, and the coalescence [3]. Though, NEs are thermodynamically unstable systems, and synthetic surfactants are often used to ensure the formation and the stability of droplets. Even so, these emulsifiers directly or indirectly raise toxicity and environment issues [4]. Hence, there is an increasing demand for natural and biodegradable products. Proteins are good candidates as emulsifiers and they are widely used to stabilize food emulsions. However, this approach is not yet applied in the pharmaceutical field. Proteins stabilize emulsions by forming a viscoelastic, adsorbed layer onto the oil droplets [5]. They are able to generate repulsive steric and electrostatic interactions between these oil droplets [6]. The aim of this study was to encapsulate curcumin within a protein-stabilized NEs for a topical application and to determine its diffusion *in vitro* through a synthetic membrane. The β-lactoglobulin (βlg), the major protein of whey, was chosen as an alternative emulsifier to replace synthetic surfactants. Results show that the incorporation of curcumin within the organic phase did not modify the characteristics of NE as well as its stability over time. Nevertheless, the stability study revealed a creaming within NEs which is a reversible phenomenon by agitation and will not be a limitation for the use of NEs. The study in Franz Cell showed that curcumin diffused slowly and could potentially have a local effect (figure1). Thus, the encapsulation of curcumin in the dispersed phase of NE seemed to be a promising strategy to increase its solubility and diffusion through a model membrane (or even the skin).

Keywords: Curcumin, Nanoemulsions, Encapsulation, protein, Franz cell, synthetic membrane.

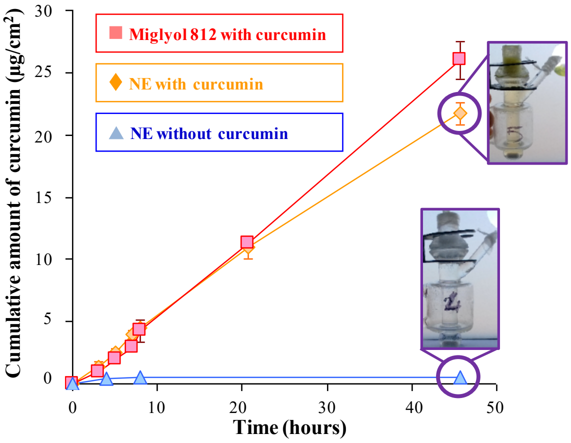

Figure 1: Time diffusion of curcumin through a synthetic membrane from different formulations: curcumin solubilized in Miglyol 812 (–) and curcumin encapsulated in NE (–). NE without curcumin was the negative control (–).

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Elaboration of the size-controlled polymeric nanomaterials; Rifampicin encapsulation and in-vitro release studies

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Abstract

The poor soluble drug family with 40% of total industry, and drugs with a continuous injection requirement for a long-term treatment has opened new opportunities for alternative drug delivery systems (DDS). Without a proper DDS the liver and other essential organs can be harmed by a continuous high-dose drug administration. In this aspect, biodegradable polymeric nanoparticles (NPs) are considered as the promising materials for DDS. NPs small size increases stability of the system in media and favors drug targeting. Small size can help escape the immune system and reduce opsonization of NPs.

The elaboration of size-controlled NPs of poly(lactic-co-glycolic) acid PLGA is studied by comparing different production techniques; sonicator, shear mixer and elongational-flow reactor and mixer (µRMX). Monomodal polymeric NPs are produced and compared. On second part, the produced NPs are employed as a nano-carrier for Rifampicin. The drug-loaded PLGA nanoparticles (DNPs) are produced at four different drug concentrations. The microfluidic encapsulation and *in-vitro* drug release micro-processes are studied. Encapsulated Rifampicin is found to decrease PLGA DNP size and it's explained on the teclis scientific technique. Techniques as dynamic light scattering (DLS), transmission electron microscopy (TEM), ultraviolent spectroscopy (UV) are employed to characterize; hydrodynamic diameter, monomodality, interfacial tension and morphology. Preferred formulation showed 65nm hydrodynamic diameter for PLGA DNPs, 42% EE, and 37.4% in-vitro drug release in 9 days by considering the drug degradation at 37°C to formulate total release quantity.

Keywords: Drug delivery systems, nanomaterials, Rifampicin, nanoparticles, encapsulation, in-vitro release

Figure 1: Interfacial tension determination on Teclis Tracker equipment before o/w nanoemulsion production.

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Co-adsorption and co-release of 5-fluorouracil and naproxen using pH-sensitive mesoporous silica particles

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Abstract:
The unfavorable physicochemical properties of many drugs affect their bioavailability and consequently the efficacy of the treatment. Drug molecules with lack of specificity and water solubility lead patients to take high doses to achieve the sufficient therapeutic effects and with frequent dosing the toxicity of the drugs increases. Dose reduction leads to drug sub-concentration and lack of therapeutic efficacy. The possible solution to maximize therapeutic efficacy and minimize side effects is to design drug delivery system which can improve the physicochemical properties of drug molecules by modifying their pharmacokinetic profile, solubility and bio-distribution. DDS is defined as a device that enables the introduction of therapeutic agent in the body and improves its efficacy and safety by controlling the rate, time and place of release of drugs in the body.

Of the various drug nanocarriers explored, stimuli-responsive end-capped mesoporous silica nanoparticles have been shown to be excellent candidates to fulfil the requirements owing to their advantageous "zero premature release" property. The drug release can be triggered by the various exogenous or the endogenous stimulus. Particularly useful one is pH change from neutral to acidic occurring in tumor tissue.

Firstly, pH-sensitive mesoporous silica nanoparticles were synthesized using amine-based stalk attached to the their walls that bind beta-cyclodextrin units non-covalently through supramolecular interactions. When the pH is decreased from its initial value, the amine derivatives become protonated resulting a binding affinity to the cyclodextrin that is decreased. The cyclodextrin caps are thus dispersed around from the stalks and pores remain un-blocked.

Secondly, we focused on the adsorption of drugs on prepared pH-sensitive system because it is adsorption phenomena that determine to a great extent the quality of pharmaceutical solid/liquid preparations. Most of the research work dealing with drug adsorption in delivery systems is essentially focused on only one adsorptive, one drug while many diseases require multiple drugs to treat them.

This work shows a comparative study of the adsorption of anti-neoplastic agent 5-fluorouracil and anti-inflammatory agent naproxen on pH-sensitive mesoporous silica nanoparticles individually and in their mixture – co-adsorption as a potential drugs delivery system.

Keywords: porous silica, functionalization, multiple drug-delivery

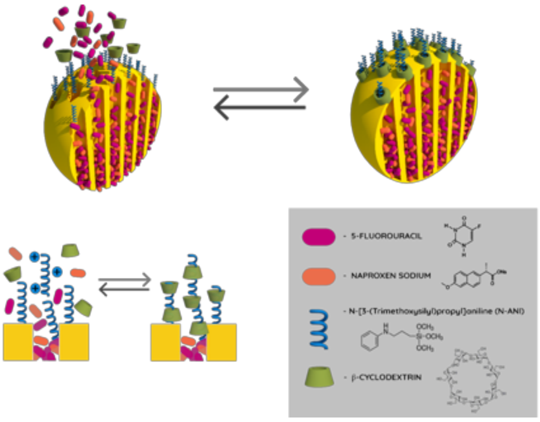

Figure 1: Schematic representation of pH-sensitive drug delivery system.

Towards Smart Drug Delivering Systems: On the Absorption of Laponite colloids onto lipid Cubosomes

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Abstract:

Due to their high water content, aqueous dispersions of lipid-based lyotropic liquid crystalline (LC) phases are excellent candidates for biocompatible applications. The addition of inorganic colloids, such as silica particles or clay platelets, allows to stabilize these systems and to form extremely stable emulsions [1-3] (Figure 1). The aim of this project is to develop new hybrid hydrogels using such a system as physical cross-linker. The position of the NPs has a key role in the cross-linking of the polymer chains. If they are absorbed onto lipid drops, they enable the linking of the emulsion to the polymeric network, on other hand, if they are free in the solvent, they can act as second cross-linker and exclude the drops from the network. An accurate characterization of the pristine emulsion is then necessary. The goal of this work is the investigation of the amount of the absorbed NPs on the lipid drops in the case of phytantriol LC phases stabilized by Laponite platelets. In this work, we propose an original method, based on the conductimetry technique, to estimate the spatial distribution of these NPs. Laponite platelets have sodium counter-ions on their surface, which can be released when the NPs are in contact with a solvent. The measure of the amount of such ions allowed quantifying how many NPs are effectively absorbed onto the phytantriol drops. The results of this study show that the necessary quantity of colloids for the stabilization of this system is very low and the majority of the platelets remains free in the solvent.

Keywords: lipid-based lyotropic liquid crystalline phase, absorption, conductimetry, Laponite nanoparticles, hybrid hydrogel.

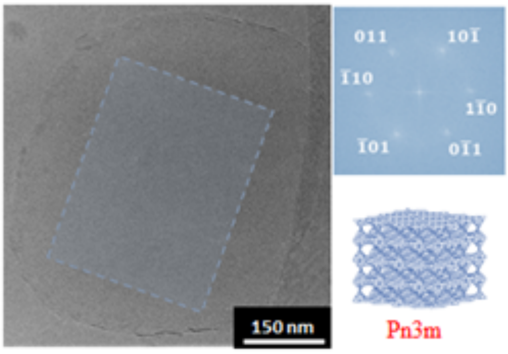

Figure 1: Cryo-TEM image of Phytantriol cubic phases stabilized by 0.5 wt% Laponite nanoparticles. The Laponite nanoparticles are clearly distinguished as small black trays.

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Poloxamer prodrug-based delivery of a pharmacologically enhanced camptothecin agent as an experimental therapy for drug-resistant neuroblastoma

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Abstract:

Poloxamers, biocompatible and water-soluble polyalkylene glycol triblock copolymers commercially available as Pluronics, offer unique advantages as the basis for macromolecular prodrug design. They are chemically and metabolically inert obviating the concern for toxic metabolites. In addition to their complete bioeliminability and absence of significant acute or delayed adverse effects, they are properly sized to provide extended blood residence, making them uniquely suited as a scaffold for creating in situ activatable polymeric prodrugs for enhancing drug delivery to solid tumors. Notably, although Poloxamers have been extensively evaluated as pharmaceutical excipients and biological response modifiers, their potential as a platform for constructing in situ activatable polymeric prodrugs with adjustable design has remained unexplored.

In our recent studies, using clinically relevant models of neuroblastoma (NB), the deadliest extracranial pediatric cancer accounting for 8-10% of all childhood malignancies and 15% of deaths from cancer in children, we showed that prodrugs formed with Poloxamers and structurally optimized topoisomerase I inhibitors of the camptothecin family can effectively treat aggressive disease refractory to conventional therapies. Poloxamer prodrug-based delivery provided enhanced uptake and achieved sustained intratumoral presence of the active drug, in turn translating into regression of chemotherapy-resistant tumors and markedly extended survival in disease models showing no durable response to conventional treatment (**Figure 1**). Importantly, the remarkable and lasting therapeutic effect of the Poloxamer-based prodrug was not accompanied by signs of systemic toxicity.

Through improving the biodistribution and enhancing the pharmacologic effect of the therapeutic cargo, Poloxamer prodrug-based delivery can potentially provide a new modality for treating high-risk NB currently lacking effective treatment options. The results of our studies can facilitate the translation of these macromolecule-linked prodrug agents as a new, clinically viable strategy for treating aggressive, drug-resistant malignancies in children and adults.

Keywords: Poloxamer, prodrug, camptothecin, topoisomerase, neuroblastoma, pediatric cancer.

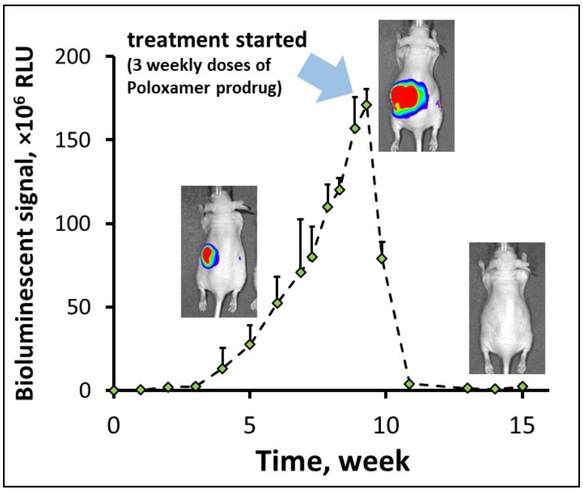

Figure 1: The antitumor effect of the Poloxamer-linked topoisomerase I inhibitor prodrug on *MYCN*-amplified tumors in an orthotopic model of high-risk, drug-resistant NB.

Acknowledgements:

These studies were made possible by support from the following sources: Solving Kids Cancer Foundation–US, Alex's Lemonade Stand Foundation, the CURE Childhood Cancer Foundation, and NIH/NCI R01-CA251883 (GMB, MC). This work was also supported by the Audrey E. Evans Endowed Chair (GMB).

Captopril-loaded polymeric nanoparticles for the treatment of pediatric diseases

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Abstract:

The Pediatric Committee at the European Medicines Agency identified the needs of the development of age-appropriate formulation of captopril in pediatric population for the treatment of cardiovascular diseases and diabetic nephropathy (1). Captopril (CAT) is currently administered by extemporaneous liquid formulation or tablet due to its limited water stability (2). Therefore, polymeric nanoparticles were developed to avoid CAT degradation and to obtain a formulation appropriate for children. Cellulose acetate phthalate (CAP) and chitosan (CH) were chosen to prepare nanoparticles by nanoprecipitation method-dropping technique without using surfactants (3). CAP nanoparticles and CAP nanoparticles combined with CH in different concentrations (1:1 w/w and 1:3 w/w) were produced both unloaded and loaded with CAT. Nanoparticles were characterized in terms of size, drug loading efficiency, physical stability during the time (1-28 days) and morphological properties. Chemical stability of drug in the dispersion was investigated. Fourier-transform infrared spectroscopy, X-ray diffraction and thermal analysis were carried out. Results show that CAP nanoparticles have no drug loading capacity, whereas CH allows the encapsulation of CAT; highest drug loading is obtained when 1:3 CAP:CH w/w ratio was used (61.28 ±6.95%). The size of loaded CAP nanoparticles is 254.86±28.57 nm, whereas that of CAP-CH nanoparticles is 248.28±35.38 nm (1:1 w/w ratio) and 433.67±20.78 nm (1:3 w/w ratio) with a PDI values around 0.2, resulting in a homogeneous system. Good physical stability of all formulations during the time is observed. At the moment, CAT appears stable in the dispersions. Spectra FTIR shows drug-polymers interactions. In conclusion, CAP-CH nanoparticles prepared using a 1:3 w/w ratio show good properties for developing suitable formulation for CAT delivery.

Keywords: captopril, polymeric nanoparticles, pediatric patients, age appropriate-formulation, nanomedicine.

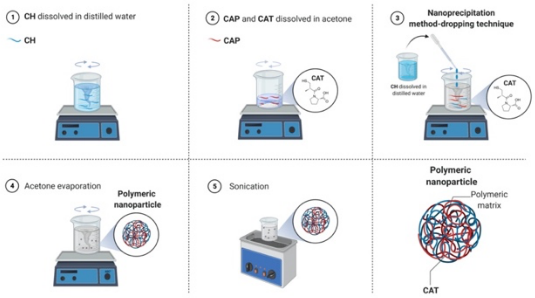

Figure 1: Figure illustrating the nanoprecipitation method-dropping technique.

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Application of Rose Bengal in the absence of light: targeting and treating melanoma via dermal delivered Rose Bengal-transfersomes

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Abstract:

Rose Bengal (RB) is a photosensitizer exhibiting intrinsic cytotoxicity towards melanoma in the absence of light, but the biopharmaceutical profile limits its clinical use. Transfersomes (TF) are ultradeformable lipid vesicles widely employed for dermal delivery of drugs as they proved to reach the deepest region of the body. Herein, we propose a transfersomal formulation of RB (RB-TF) to target and treat melanoma via dermal delivery in the absence of light. RB-TF (RB=500 μM), were prepared by a modified reverse-phase evaporation method employing Lipoid S100, cholesterol and Span®80 as lipid. RB-TF were 200 nm-sized and homogenously dispersed; the zeta potential value was below -30 mV. Stability studies proved that a storage period of 60 days did not considerably perturb the dimensional properties and the RB content of RB-TF; RB-TF protected RB from photodegradation when exposed to visible light over 24 hours. The spectrophotometric and fluorimetric, SAXS and morphological investigations revealed RB efficiently interacted with the lipid phase; indeed, RB intercalated within phospholipid bilayer originating unilamellar and ultradeformable vesicles, whereas corresponding empty TF displayed a rigid multilamellar structure. Besides, the ex-vivo epidermis permeation study demonstrated that RB-TF significantly increased RB's amount permeating the epidermis compared to the free drug (78.31% vs 38.31%). Antiproliferative assays on melanoma cells suggested that RB-TF effectively reduced cell growth compared to free RB at the concentrations tested (25 and 50 μM), and RB-TF could potentially increase selectivity towards cancer cells. Considering the outcomes of characterization and cytotoxicity studies performed on RB-TF, and considering that melanocytes reside in the epidermis or deeper in the dermis, RB-TF can potentially treat melanoma in the absence of light via dermal delivery.

Keywords: Rose Bengal, transfersomes, liposomes, lipid-based nanoparticles, dermal delivery, skin delivery, melanoma.

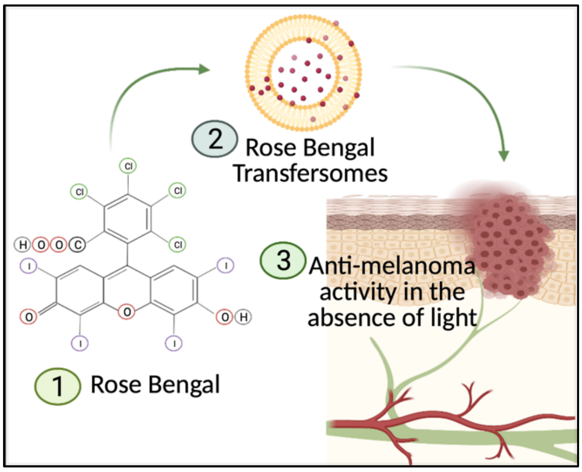

Figure 1: The figure graphically resumes the aim of the current work. Rose Bengal, an amphiphilic photosensitizer, is encapsulated in transfersomes to treat melanoma lesions in the absence of light, exploiting the dermal administration route. Created with BioRender.com.

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Scrutinizing nanoparticle-membrane interactions: Effects of the biomolecular corona, particle size and flow

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Abstract:

Nanoparticles show promise as drug delivery vehicles due to their design possibilities and cancer targeting capacity. However, a clear view on the parameters that affect uptake is still lacking. To lay bare the mechanisms that govern particle internalisation, studies of the physical interactions at the first point of contact between particles and cells are necessary. In this work we focus on the adsorption of nanoparticles to model cell membranes. Emulating the *in vivo* environment is important as both chemical and physical aspects influence particle-membrane interactions. One example is the presence of a biomolecular corona, the layer of adsorbed biomolecules that cover pristine particles once introduced into the blood stream. Using total internal reflection fluorescence microscopy and lipid bilayers as a model membrane system, we systematically studied the adsorption and residencey of nanoparticles on membranes under controlled conditions (Figure 1). The effect of particle size, biomolecular corona and flow on particle adhesion were studied. A clear effect of the biomolecular corona was found; the probability that particles resided for longer times decreased significantly for particles covered with various degrees of corona compared to bare particles. This inhibition of strong adsorption is consistent with the general idea of corona formation "passivating" the bare nanoparticle surface. All particle sizes exhibited mainly transient interactions under full corona conditions with only a few events of extended duration. Finally, the addition of flow resulted in a decrease of the number of adsorption events, highlighting the importance of physiological flow conditions for nanomedicine studies.

Keywords: nanomedicine, nanoparticles, lipid bilayers, membrane, adhesion, biomolecular corona, flow, total internal reflection microscopy, drug delivery applications.

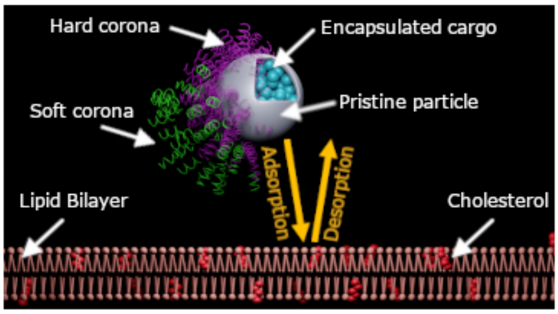

Figure 1: Graphical depiction of a nanoparticle adsorption-desorption event on a model membrane. In biological environments the surrounding biomolecules adsorb onto the pristine particle surface forming a strongly bound hard corona and transiently bound soft corona. The adhesion to the membrane of the resulting particle complex is goverened by biomolecule-lipid bilayer interactions.

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Novel applications of nanobiotechnology to decipher cell-materials and cell-cell interactions

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Abstract:
Nano-materials can interact with cells to guide their organization and assembly into structures, with functionalities that support, improve or replace those displayed by biological tissues or organs, with applications in tissue engineering, biocomputing, cell-based sensors, diagnosis and analysis of pathologies and of drug efficacy.

Using nanotechnology and advanced sensitive materials, we produced devices in which the topography of the substrate is controlled at the nanometer level to influence and guide the organization of single neural cells in clusters forming complex networks. In doing so, combining direct experiments with computer simulations and mathematical modelling, we studied how (i) the geometry of the surface can change the topological properties of the cells, (ii) the topological properties and number of elements in the system may affect and possibly improve the quality, density and spread of information throughout a network of cells and (iii) whereby cells create networks which minimize energy consumption [1–6]. This knowledge can be applied to decipher the mechanisms through which the brain marshals its millions of individual nerve cells to produce behavior and, ultimately, reveal the circuits responsible for neurodegenerative disorders in that neurodegeneration can be regarded as a connective failure affecting information.

In addition, we designed, fabricated and characterized various matrices embedding optical ratiometric microparticles sensors[7–9] for the measurement of cellular metabolism-related analytes, such as oxygen and pH, during cell growth and tissue formation.

In particular, we developed additive manufactured 3D scaffolds embedding capsules-based optical sensors and demonstrated the potential of these integrated systems by calibrating and monitoring in space and time pH variations of human mesenchymal stromal cells (hMSCs) in different areas of the constructs (Figure 1).

The research leading to these results received partial funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 759959, ERC-StG "INTERCELLMED").

Keywords: nano-topography, microparticles, pH mapping, tissue engineering.

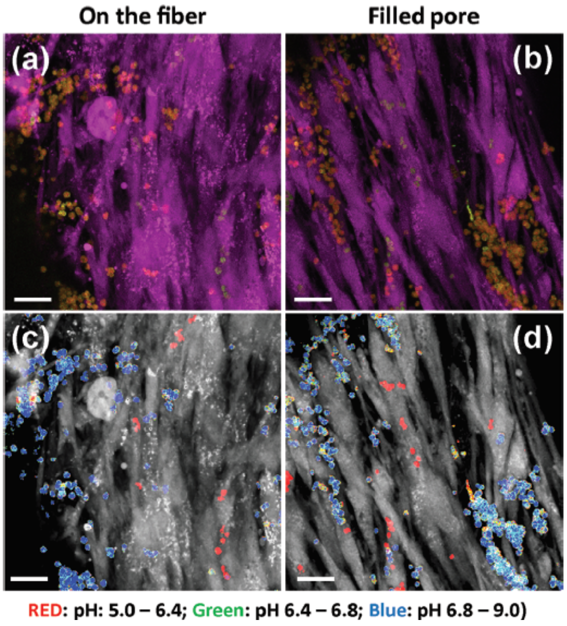

Figure 1: Maximum intensity z-projection images representing hMSCs and pH-sensing capsules. a,c) Capsules sensing pH around cells growing on the fiber and b,d) capsules sensing pH around cells in the filled pore of the 3D scaffold (day 7). (a, b) Intensity-based images. Magenta: Cytoplasm (calcein). Green and red correspond to the signal of the pH-sensitive capsules. (c,d) pH images. In these images the cytoplasm coding is converted to gray for better clarity and the red, green, and blue coding indicates different pH ranges. Scale bars: 20 µm.

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Posters Abstracts

Synthesis of Stretchable and Environmentally Stable Conjugated Polymer PEDOT using a Random Copolymer with Modified Acid Template

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Abstract:

Although Poly(3,4-ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT:PSS) has good electrical conductivity and high transparency in most applications, its usage in stretchable applications is limited because of its rigidity, reduced conductivity after elongation, and poor environmental stability. This study addresses these issues by incorporating the soft and relatively hydrophobic moiety poly(ethylene glycol) methacrylate (PEGMA). By incorporating PEGMA randomly in the rigid PSS chain, a soft and hydrophobic copolymer P(SS-co-PEGMA) is obtained. The conducting P(SS-co-PEGMA)-based polymer-coated PET film exhibits good resistance even after 400% elongation. In addition, PEDOT:P(SS-co-PEGMA) has better environmental stability than PEDOT:PSS because of the presence of the relatively hydrophobic PEGMA moiety in the chain. Moreover, the potential applicability of the synthesized flexible and stretchable electronic material as a stretchable matrix is established, which includes inorganic conductors(AgNW). When this material is stretched, it can be applied as a conductive interconnector to maintain the electrical pathway, instead of the other insulating matrices.

Keywords: Stretchable conducting polymers, random copolymers, PEDOT:PSS, PEDOT:P(SS-*co*-PEGMA), electrical interconnector

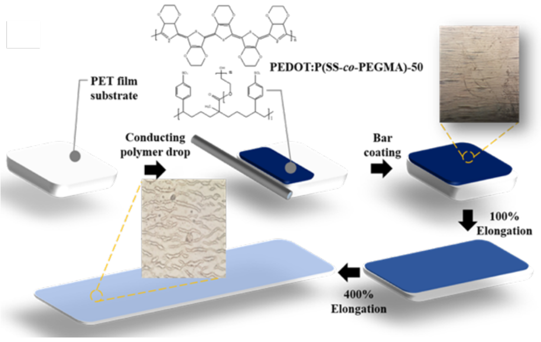

Figure 1: Figure illustrating the molecular structure of intrinisically stretchable conducting polymer PEDOT:P(SS-*co*-PEGMA) and the 400% elongation of PEDOT:P(SS-co-PEGMA).

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Optical properties and enhancement of Raman scattering of gold nanostructured arrays elaborated by scanning probe lithography

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Abstract:

Gold nanostructured arrays obtained by scanning probe lithography is a powerful tool for Surface Enchancement Raman Spectroscopy (SERS) analyses [1]. As previously reported, different nanostructures can easily be elaborated on the same substrate, by varying height, width, spacing between structures. The modification of topography can induce variations of optical properties and SERS efficiency as well. So, the present work was mainly devoted to predict, in the visible range, the optical response of the supports and compare the results to the experimental absorbances. Regular arrays of gold 3d-nanostructures were elaborated folowing the methodology reported previsouly [1]. Height has been fixed to 110 nm and spacings varied between 0 to 360 nm. The topographical characterization of the surface was performed by atomic force microscopy (AFM) in order to record the profil of each nanostructure at nanoscale. The near-field enhancement studies were performed by finite element analysis using wave optics physics in COMSOL Multiphysics®. Our model was set up with two domains : the gold film was modelled using the Lorentz-Drude dispersion model and the above medium was defined as air [2]. Figure 1 shows the results of simulated absorbance as a function of wavelength. Absorbance decreases with increasing spacing.

Experimentally, we recorded the reflectance of the nanostructured support by using brightfield microscopy and determined the extinction spectra for each structure. Our results showed a well-defined bands for structures with small spacing and a more complex specral response when spacing increases. Let us note that both simulated and measured extinction intensity decrease with increasing spacing, suggesting that the SERS may be impacted. So, Raman imaging has been carried out at $\lambda = 660$ nm on the different structures after immersion in a 10^{-6} M solution of thiophenol. In Figure 2, SERS intensity decreases with increasing spacing, as revealed by the normalized Raman intensity maps (inset of the Figure 2).

Keywords: gold nanostructures, COMSOL, Raman, SERS, extinction, scanning probe lithography.

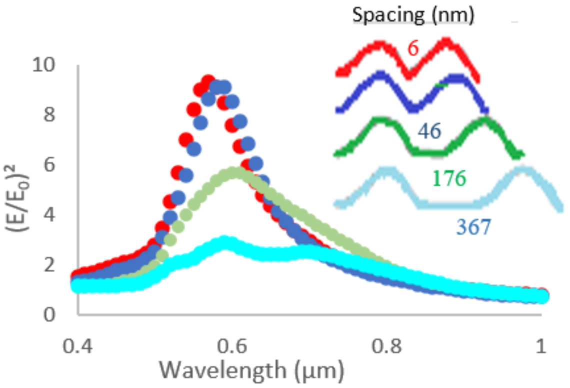

Figure 1: Simulated extintion spectra for different spacings. Height was fixed to 110±10 nm.

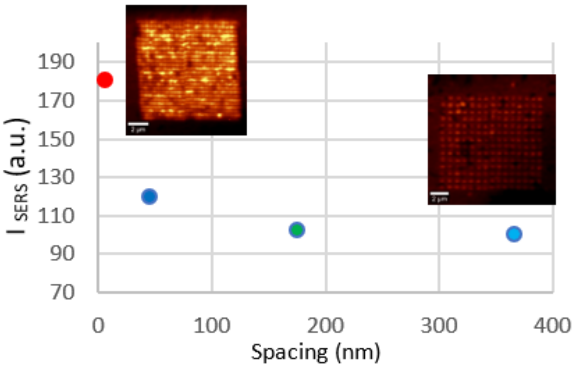

Figure 2: SERS Intensity evolution as function of spacing. Inset: Normalized Raman intensity mappings (12x12 μm^2) of 14 400 spectras ($\lambda = 660$ nm, P= 2 mW, t= 2s), with spacing of 6 and 367 nm.

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The effect of nanofiller on the production of high performance multi-layer fine-fibrous filter material by application of fused deposition modeling

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Abstract:
Mixing of polymers is an effective method of enhancement of physical, chemical and performance characteristics. The properties of such systems are determined by their structure, the formation of which is associated with miscibility or immiscibility of the components, as well as with the processes of deformation, decomposition, and coalescence of droplets of the dispersed polymer phase under mixture conditions. Until recently, the immiscibility of components was considered a significant drawback of such blends, however, in many cases, due to the multiphase nature of the polymer dispersions, materials based on them have unique performance characteristics. The decisive factor in creating fibrillar heterogeneous morphology in polymer blends is the immiscibility of their components. The morphology of immiscible blends depends on many factors: composition, relative viscosity of the components, surface tension at the interface, thermodynamic instability, mixing time and speed, geometry and dimensions of the extruder screw, etc. The introduction of a compatibilizer into the blend leads to increased interaction between the phases and the formation of a finer stable dispersion. Nanoadditives can also causes a compatible effect, which helps to improve the dispersion and stability of the despersed phase, as well as the formation of fibers of one polymer in the matrix of another.

The effect of the nanofiller on the rheological properties, interfacial phenomena, and the morphology of polypropylene/copolyamide (PP/CPA) blends was studied. It was shown that the addition of carbon nanotubes (CNTs) and zirconium dioxide (ZrO_2) slightly decreased the melt elasticity of the initial PP and increased its viscosity. As a result, in the modified blends, the viscosity ratio (the ratio of the viscosity of the matrix to the viscosity of the dispersed phase) and elasticity ratio (the ratio between the Weissenberg number of the droplet phase and matrix) were close to 1, which contributed to better dispersion of PP and the formation of PP nanofibers in the CPA matrix. In nanofilled blends, the process of fibre formation of PP in the CPA matrix was improved as a result the average diameter of microfibers was reduced from 910 nm (for the original blends) to 640 nm and 580 nm for ZrO_2 and CNT based composites, respectively.

Keywords: fused deposition modeling, nanoadditive, multi-layer fine-fibrous filter material, in situ formation of nanofibrillar composites.

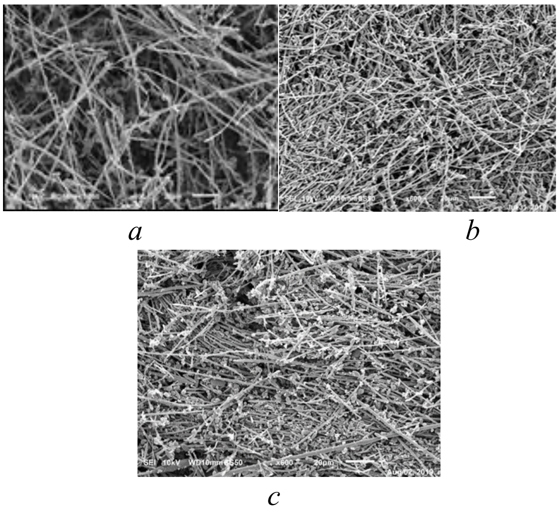

Figure 1: SEM images of surfaces of PP/CPA (*a*), PP/CPA/2,5 wt.% ZrO_2 (*b*) and PP/CPA/2,5 wt.% CNT (*c*) composites after CPA extraction.

Acknowledgments: The project was financed from funds of the National Science Centre (Poland) on the basis of the decisions number DEC-2017/25/B/ST8/02059.

Morphology, Thermal and Mechanical Properties of Polylactide Blends with Glycidyl Methacrylate-grafted Polypropylene

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Abstract:
Polylactide (PLA) is a thermoplastic aliphatic polyester derived from renewable resources such as corn, cassava, sugarcane, etc. However, the brittleness of PLA limits its practical applications in various commodity sectors. Polypropylene (PP) as a petroleum-based thermoplastic polymer is widely used in commodity goods, due to its cost-effectiveness, good mechanical toughness and satisfactory heat resistance. However, PP is not miscible with PLA. On the other hand, glycidyl methacrylate (GMA) has been chosen as a reactive compatibilizing agent for polyolefins such as PE and PP. Therefore, it is expected that glycidyl methacrylate-grafted PP (PP-g-GMA) can be utilized as a polymeric compatibilizer to enhance the physical properties of pristine PLA. In this study, PP-g-GMA was fabricated by free-radical grafting of GMA onto PP backbone via reactive melt-compounding and a series of PLA/ PP-g-GMA blends were also manufactured via efficient melt-compounding. The morphology, rheological, thermal and mechanical properties of PLA/PP-g-GMA blends were investigated by using FT-IR, SEM, rheometer, DSC and DMA. The influence of PP-g-GMA on the structure and properties of PLA was analyzed by considering the PP-g-GMA content and the specific interaction between PP-g-GMA and PLA. The SEM images confirmed that the neat PLA had a smooth surface due to its brittle fracture, and that PLA/PP blend exhibited the phase separation structures. However, PLA/PP-g-GMA blend showed a relatively uniform and ductile fractured surface without any phase-separated domains. The DSC analyses of PLA/PP-g-GMA blends revealed that both the cold-crystallization of PLA component and the melt-crystallization of PP component occurred at lower temperatures. It demonstrates that the melt-crystallization of PP-g-GMA was retarded, while the cold-crystallization of PLA was accelerated by the nucleating effect of PP crystals.

The FT-IR spectra confirmed the presence of the chemical reactions as well as specific interactions between the epoxy groups of PP-g-GMA and the hydroxyl and carboxylic groups of PLA during the melt-compounding. The DMA results indicated that, as the PP-g-GMA content increased in the blends, the storage moduli at the glassy temperature range below ~60 °C decreased owing to the enhanced flexibility of the blends. The shear moduli of PP-g-GMA were measured to be lower than those of neat PP because of the GMA grafting effect on PP chains. However, the shear moduli of PLA/PP-g-GMA blend were far higher than those of PLA/PP blend, which is related with the improved compatibility due to the chemical reaction and specific interaction between PLA and PP-g-GMA during the melt-compounding Overall, it was found that the high brittleness, low toughness, and slow crystallization of PLA can be improved effectively by the incorporation of PP-g-GMA component as a reactive compatibilizer.

Keywords: Poly(lactic acid), Polypropylene, Glycidyl methacrylate, Compatibilizer, Melt compounding.

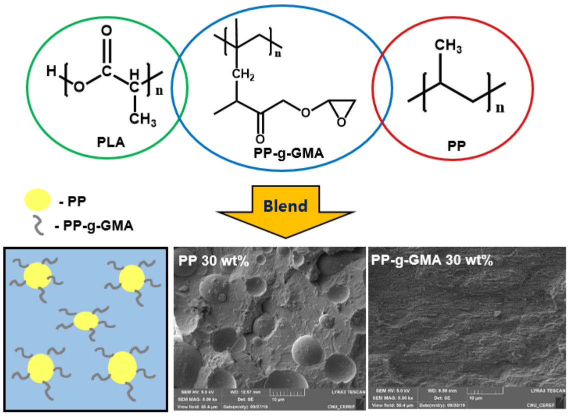

Figure 1. Morphologies of PLA/PP and PLA/PP-g-GMA blends.

Thermally Conductive Polyimide-based Composites Films with Low Dimensional Ceramic Nanofillers

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Abstract:
As electronic devices become smaller and higher performance, heat generation is becoming an important issue. Accordingly, a demand for materials capable of efficiently and rapidly releasing heat keeps increasing. The commonly used thermally conductive fillers for polymer composites can be categorized into metallic and ceramic fillers. The metallic fillers, such as copper nanoparticles, copper nanowires, silver particles, gold and palladium powders could be used to enhance the thermal conductivity of a polymer composites. However, these metallic fillers may lead to an increase of electrical conductivity, which limits their practical applications for electronic devices requiring electrical insulation. In the study, ceramic fillers such as 1-dimensional silicon carbide (SiC) and 2-dimensional boron nitride (BN) sheets have been used as thermally conductive nanofillers for polyimide (PI) film because of their high thermal conductivity and electrical insulation property. For the purpose, poly(amic acid) as a precursor of PI film was synthesized by using 3,3',4,4'-biphenyltetracarboxylic dianhydride (BPDA) and 4,4- oxydianiline (ODA). A series of PI-based composite films containing different conents of SiC or BN were fabricated by using solution casting and following heat treatment. The molecular and morphological structures of the composite films were characterized with aids of FT-IR and SEM. The thermal stability, thermal conductivity, and mechanical property of the composite films were investigated by using TGA, LFA, and DMA, respectively. Due to high modulus of SiC and BN fillers, the storage modulus of the composite films increased with increasing the filler content in the composite film. The thermal conductivity of the composite films increased with increasing with the filler content in both in-plane and out-of-plane directions.

Keywords: Polyimide, Boron nitride, Silicon carbide, Thermal conductivity, Thin films, Solution casting.

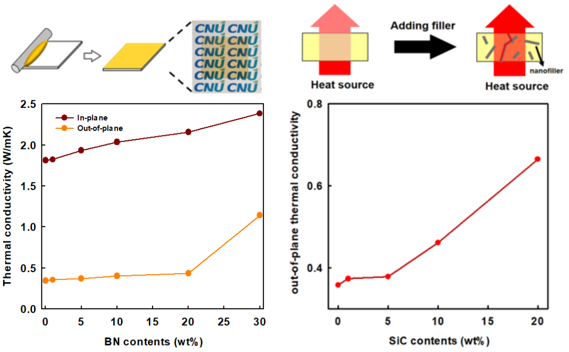

Figure 1: Scheme for fabricating polyimide-based composite films with silicone carbide or boron nitride fillers.

Aromatic Poly(ether amide)s-derived Carbon Nanofiber Webs for Self-standing and Binder-free Supercapacitor Electrode Materials

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Abstract:

Electrospinning is known to be a versatile and facile process to fabricate continuous carbon nanofibers (CNFs) in large quantities at a low cost. A variety of polymeric precursors, such as polyacrylonitrile (PAN), polyimide (PI), polybenzimidazole (PBI), poly(vinyl chloride) (PVC), etc., have been thus investigated to prepare electrospun and activated CNFs via heat-treatment and chemical/physical activation processes for potential applications as electrode materials of energy storage devices. In this study, we have synthesized aromatic poly(ether amide) (PEAs) by using a phosphorylation-based polycondensation reaction. The synthesized PEAs were found to exhibit good solubility in organic solvents such as NMP, DMSO, and DMAc and to have excellent thermal stability with high char yield above 60% at 800 °C. A series of CNFs were fabricated by electrospinning of mixed solutions of PEA and poly(vinyl pyrrolidone) (PVP) at different ratios, followed by carbonizing the as-spun nanofibers at 100 °C. The microstructural features of PEA/PVP-derived CNFs were characterized with aids of SEM, EDS, FT-IR, Raman, and XRD. The electrical and electrochemical properties of the CNFs were analyzed by using conductivity measurement, cycle voltammetry (CV), galvanostatic charge-discharge (GCD) test, and electrochemical impedance spectroscopy. The SEM and Raman data revealed that PEA/PVP-derived CNFs with the quasi-ordered graphitic structure were successfully fabricated. The electrical resistivity of the CNFs was evaluated to be in the range of 0.03-0.09 Ω cm, which results from the electrically conductive graphitic structure developed during the carbonization. The specific capacitance of CNFs was 537.2 A/g at 5 mV/s due to improved electrical conductivity, improved specific surface area. High specific capacitance and operational stability of PEA/PVP-derived CNFs were verified through the three-electrode system. It is thus reasonable to contend that PEA/PVP-derived CNFs can be utilized as highly stable, self-standing and binder-free electrode materials for wearable energy storage devices.

Keywords: Aromatic poly(ether amide), Carbon nanofibers, Electrospinning, Electrochemical property, Electrode materials

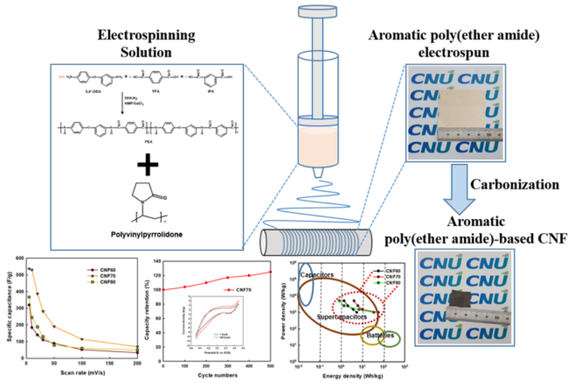

Figure 1. Schematic illustration to prepare aromatic poly(ether amide)-derived carbon nanofibers (CNFs) for supercapacitor electrode materials.

Preparation and characterization of carbon containing composite films on Al-Zn-Mg alloy using steam coating

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Abstract:
Fuel cells are expected as next energy devices. Separator is one of the most important parts in the fuel cell. Carbon and steel have been used as material for separator. Recently, the demand for the separator with lightweight and high strength has been increasing and superior corrosion resistance against acidic environment has been also required. From the viewpoint of these, aluminum alloys have been focused as parts of next separator. In addition, Al-Zn-Mg alloy has attracted much attention because of the lightweight and high strength. However, the presence of Cu and other additive elements needed to increase the strength of an alloy decrease their corrosion resistance, making it necessary to find ways to improve this corrosion resistance. In addition, conductivity is also required to use as separator. Therefore, it is desirable to develop new surface preparation techniques for improving the corrosion resistance and conductivity of Al-Zn-Mg alloys. In this presentation, we report the preparation of corrosion resistance and conductive composite films by a novel steam coating process using carbon materials. Steam coating is a process that causes metallic hydroxides and oxides to form on the surface of an alloy through the reaction of steam with the metal inside an airtight reaction vessel. Since it does not use harmful chemicals or, like anodic oxidation, require a large amount of power, the environmental impact of steam coating is low.

Corrosion resistant and conductive films were prepared on Al-Zn-Mg alloy by steam coating process using carbon materials such as graphite and carbon nanotube. X-ray diffraction patterns and SEM images demonstrated that carbon containing AlO(OH) film was formed on the Al-Zn-Mg surface by steam coating. The corrosion resistance of the film in sulfuric acidic aqueous solution at pH = 3 was investigated by potentiodynamic polarization curve measurements.

All films prepared by steam coating had crystalline AlO(OH) phase and were realtively dense. Figure 1 shows potentiodynamic polarization curves of graphite, or cup stucked cabon nanotube (CSCNT) containing composite films in surfuric acidic aqueous solution at pH = 3. The anodic current densities of all film coated samples decreased considerably, compared to untreated Al alloy, indicating all films can provide superior corrosion resistance to Al alloy.

Keywords: Corrosion resistance, Acid resistance, Resistivity, Aluminum alloy, Separator.

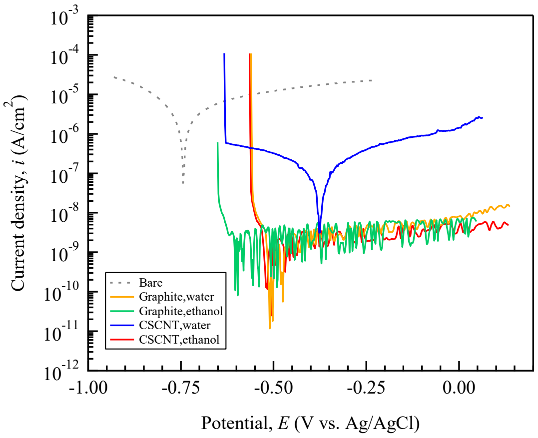

Figure 1: Potentiodynamic polarization curves of graphite, or cup stucked cabon nanotube containing composite films in surfuric acidic aqueous solution at pH = 3.

Acknowledgment: T This research was supported by Japan Science and Technology Agency (JST) under Program on Open Innovation Platform with Enterprises, Research Institute and Academia (OPERA) (No. 18072116).

Synthesis and Characterization of Cu2S – TiO2 Heterostructures with Enhanced Photophysical Properties.

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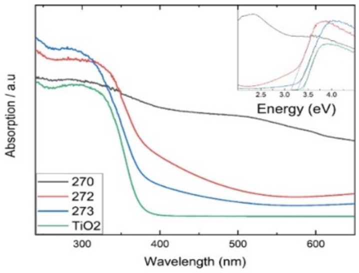
Abstract:

As environmental damage continues to increase with time, research must be conducted with environmental applications in mind. TiO_2 has been extensively studied for photocatalysis due to its feasible synthesis as well as its chemical and thermal stability. A main drawback of TiO_2 is its large bandgap, which leads to its poor photocatalytic activity in visible light. This can be overcome by using TiO_2 in conjunction with low bandgap semiconductors. Recent studies proved that doping TiO_2 with copper-based material has shown to display better photocatalytic activity in visible light than pure TiO_2[1,2]. In this study, we synthesized $Cu_2S@TiO_2$ nano-heterostructures of different copper ratios utilizing the sonochemical method. The composites were characterized using numerous techniques. The use of the Scanning Electron Microscope showed the preservation of the structural integrity of the TiO_2. Powder X-Ray Diffraction and Raman Spectra confirmed the presence of both materials and their crystalline nature. UV-Vis proved the capability of Cu_2S to enhance the light absorption of $Cu_2S@TiO_2$ towards the visible region with a decrease in the bandgap up to 3.1eV. Previous research has shown the application of TiO_2 for water splitting and chemical degradation via photocatalysis[3,4]. Sulfur doped copper nanoparticles exhibited promising applications towards a selective reduction of CO_2 to formate[5,6]. Thus, the newly developed $Cu_2S@TiO_2$ nanocomposite has great promise of application for water splitting and CO_2 reduction. Consequently, helping the cause of decreasing environmental damage.

Keywords: Heterostructures, composites, CO_2 reduction, water splitting, photocatalysis, environmental damage, sonochemical method.



UV-Vis spectra of unmodified TiO_2, Cu_2S (270), and Cu2S@TiO2 (272,273) with varying ratios of Cu2S and TiO2.

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Impact of pH on adsorption of hydrogen on Pt in aqueous phase

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Abstract:

Dissociative adsorption of H_2 is the first elementary step in hydrogenation and hydrogenolysis on metal reactions, involving H_2 physisorption, cleavage of H-H bond and formation of H-metal bond.[1] The heat of adsorption of H_2, also interpreted as hydrogen binding energy (HBE), is sensitive to the acid-base properties of the surrounding environment.[2] However, the mechanism is still under debate in electrochemistry,[3] by reason of a pH-dependent behavior of water at Pt-H_2O interface or a change in the near-interface ions.[4] This work determined the adsorption heat for H_2 on carbon nanotube supported Pt nanoparticle (Pt/CNT) with variation of pH in aqueous phase in the absence of electrolyte and under a high pressure of H_2. A kinetic method is established to determine the thermodynamic properties of adsorbed H atoms through the adsorption of H_2 (g) on Pt/CNT in D_2O (l) with variation of pH, by monitoring the formation rate of HD and D_2. The reactions of H_2 (g) with D_2O (l) into D_2 (g), HD (g) and HDO (l) on Pt/CNT involves adsorption of H_2 on Pt and desorption of H_2, HD and D_2. Measuring the adsorption and desorption rates and corresponding activation energies of adsorption and desorption enables the determination of the adsorption heat by their difference (Figure 1(a)). In the elementary steps, H_2 dissociates into H atoms on Pt surface and partially exchange to D atoms with D_2O. The H and D atoms recombine into HD, H_2 and D_2 desorbing from Pt surface. Under a certain pressure of H_2, the formation rate of HD (r_{HD}) and D_2 (r_{D2}) are measurable in the reaction, while that of H_2 (r_{H2}) is calculable using r_{HD} and r_{D2}. Figure 1(b) shows the activation energy of adsorption and desorption as well as the heat of adsorption of H_2 in water. The adsorption heat decreases from 45 to 38 kJ mol^{-1} with pH decreasing from 7 to 2, reflecting that the concentration of hydronium ions has a significant influence on dissociative adsorption of H_2 on Pt. There is almost no activation barrier (1 kJ mol^{-1}) for the adsorption of H_2 on Pt/CNT at pH 7, which is consistent with previous study that dissociative adsorption of H_2 on Pt is spontaneous.[5, 6] However, the activation energy of adsorption starts rising up from 1 to 8 kJ mol^{-1} with pH declining from 7 to 2, while the activation energy of desorption keeps constant during the whole measured range of pH. This is hypothesized to be a consequence of the dense layer of hydronium ions at the surface of Pt at low pH, which builds up an additional barrier for H_2 to approach to Pt surface.

Keywords: Dissociative adsorption of H_2, Pt catalyst, carbon nanotube, hydronium ions, aqueous phase.

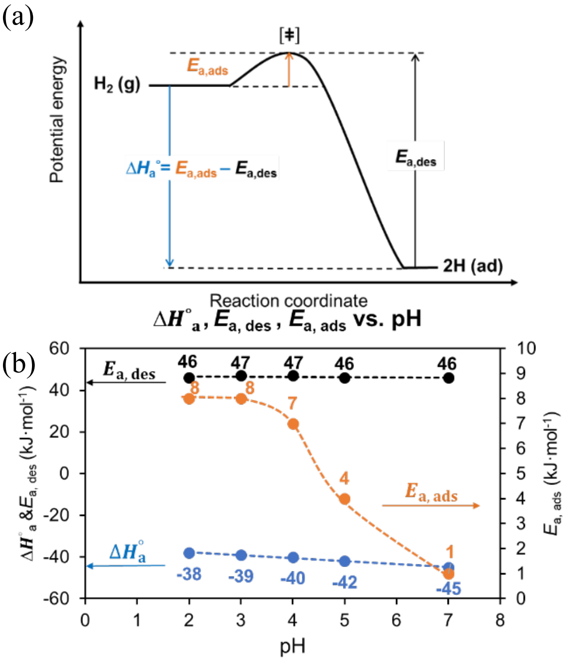

Figure 1: (a) The energy diagram of dissociative adsorption of H_2 on Pt/CNT in water, and (b) impact of pH on ΔH_a° (enthalpy of adsorption), $E_{a,des}$ (activation energy of desorption) and $E_{a,ads}$ (activation energy of adsorption).

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Optically Mapping Temperature in the Vicinity of Gold Nanorods

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Abstract:

When gold nanorods (AuNRs) are irradiated with light of a frequency that matches their resonance frequency, the light is efficiently absorbed. Almost all of this energy is converted into heat by non-radiative processes and is subsequently locally dissipated [1]. This is called the photothermal effect. For gold nanorods the wavelength at which this occurs is in the near infrared region of the spectrum. Near infrared light can penetrate through soft tissue and thus this photothermal effect could be adopted for future cancer treatments, where the local heating from the irradiated gold nanorods results in cancer cell death. Accurate temperature measurement in this regime is difficult, since we are dealing with the critical dimension such as single cell. Few studies have been conducted on direct measurements of local temperature associated with irradiated AuNRs in a biologically relevant context. Luminescence thermometry is a promising technique for measuring the temperature in tissues. Recent studies have shown quantum dots (QDs) to be sensitive to temperature and able to report temperatures variation. Here we present AuNRs that are coated with silica shell to resist shape change under laser irradiation, decrease toxicity of CTAB, protect AuNRs from aggregation and make them thermodynamically stable [2]. The AuNRs/silica will be incorporated with QDs which will provide stable fluorescence tracking and temperature measurement capability to the AuNRs in the cells.

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Structural analysis of AlInN layers deposited on Si(100) and Si(111) via reactive RF sputtering

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Abstract:
III-nitride materials (AlN, GaN, InN and their ternary alloys) have gained a great interest in the last two decades due to their application in visible-NIR optoelectronic devices. The wide bandgap energy of $Al_xIn_{1-x}N$ can be tuned by changing the alloy composition, x. However, the challenge of growing high quality single phase $Al_xIn_{1-x}N$ films relies on the differences in the properties of its binary constituents, InN and AlN. Different techniques have been reported for growing $Al_xIn_{1-x}N$ layers, such as metal-organic vapor deposition, molecular beam epitaxy and radio-frequency (RF) sputtering. The latter allows the deposition of III-nitrides over large areas and at lower substrate temperatures, at the expense of a higher defect density.

In this work, we examine the structural properties of three $Al_xIn_{1-x}N$ on Si samples with an Al content of $x = 0.36$ deposited via RF sputtering. The layers were deposited at low temperature (300ºC) on Si(100) and at high temperature (550ºC) on Si(100) and Si(111) substrates, to study the effect of the growth temperature and substrate orientation on their structural properties. The deposition was carried out with a pure nitrogen flow of 14 sccm and a pressure of 0.47 Pa [1]. The RF power applied to the targets were 150 W for Al and 30 W for In. A detailed study of the structural and morphological quality of the layers was carried out through high-resolution X-ray diffraction (XRD), atomic force microscopy (AFM), high-resolution transmission electron microscopy (TEM) and energy-dispersive X-ray spectroscopy (EDX).

From the X-ray diffraction pattern θ-2θ we obtain the Al mole fraction using Vegard's law and assuming fully relaxed layers. We also observe no phase separation and a low value of the FWHM rocking curve (~5º), indicating a low mosaicity of the layers. On the other hand, the rms surface roughness obtained from AFM images remains ~ 2.4±0.3 nm for layers grown on both Si substrates and at both temperatures. A film thickness of ~190 nm is measured for all samples through TEM images. Moreover, the presence of an amorphous layer of ~2.5 nm between the substrate and the material is also found in all samples. From the Fast Fourier Transform (FTT) of the diffraction pattern, we can observe a compact and highly-oriented c-axis crystalline structure aligned with the substrate crystalographic orientation. Finally, compositional analyses performed by EDX reveal the presence of nitrogen and oxygen in the amorphous interfacial layer found between the nitride and the Si substrate.

The high quality of the samples is preserved when growing on both Si(111) and Si(100) substrates. At the same time, the high substrate temperature promotes the incorporation of oxygen into the amorphous layer.

Keywords: AlInN, RF sputtering, XRD, AFM, TEM, EDX, amorphous layer, Si(100), Si(111).

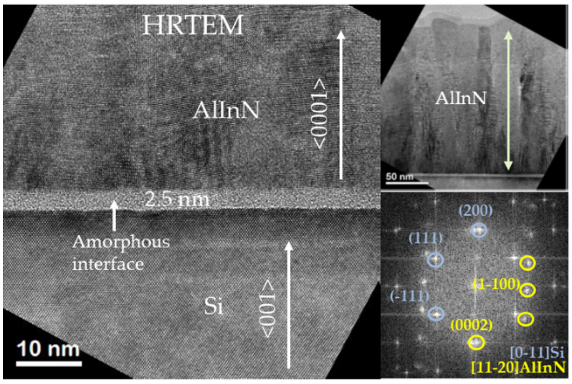

Figure 1: High-resolution TEM image and FTT of $Al_xIn_{1-x}N$ grown on Si(100) at 300ºC.

Acknowledgements: we thank projects SOLA (CM/JIN/2019-013), NERA (RTI2018-101037-B-I00), SINFOTON2-CM (P2018/NMT-4326).

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Recording Material Synthesis Images and Processing with a Script for Data Visualization

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Abstract:

Chemical synthesis is ubiquitous as the foundation for material fabrication, including nanomaterials. Control over these syntheses is of paramount importance. With the aid of Python, a programming language, a script was developed to process videos or a sequence of images, which are then processed into a graphic with three color channels, red, green and blue, as a function of time. Such a simple output can reveal a plethora of information, such as the temperature at which a precipitation, reaction or phase change occurs. The data graphic of a synthesis can also be compared with a replica of the same synthesis to ascertain if reproducibility was achieved. The applicability of this script includes any sort of synthesis where recording images is possible, even with a mobile phone camera. A series of metal sulfide semiconductor nanomaterials synthesis color profiles will be presented, such as copper sulfide and cobalt sulfide, as examples, as some of the intrinsic limitations of the method and expandable features of the data acquisition method.

Keywords: feature extraction, imaging, recording, reproducibility, synthesis

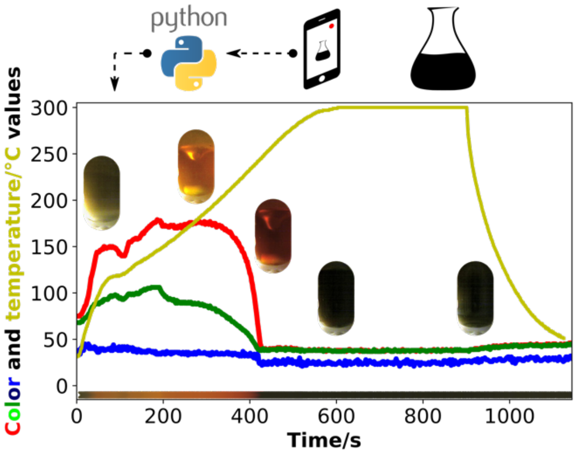

Figure 1: Graphic with a color and temperature profiles of a copper sulfide nanoparticle synthesis performed in a microwave reactor. The data was acquired by recording images during the synthesis and processing with a Python script, as depicted on the scheme above.

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3D-printed Bioactive Scaffolds for Bone Regeneration Bearing Carbon Dots for Bioimaging Purposes

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Abstract:

Additive manufacturing, or else 3D printing, has been successfully employed to create novel bioactive scaffolds incorporating carbon dots for additional bioimaging. Fused filament fabrication technique was used to print a hybrid poly-lactic acid (PLA)-based filament bearing bioactive material for hydroxyapatite (HA) development and carbon dots for additional imaging of the process. The technique and the biodegradable PLA can be used to create the exact tailored-made scaffold depending on the needs (i.e. shape of a bone fracture), whereas the bioactive material (i.e. bioglass® 45S5 or porous calcium oxyboroapatite) assists bone regeneration by HA development [1,2]. A 3D-printed wrist scaphoid bone analog bioactive scaffold is shown in Figure 1. On the other hand, biocompatible red emissive boron-doped carbon dots allow the procedure monitoring. Scaffolds were tested for their biodegradability and bioactivity in proper simulated body fluids. Degradation of the PLA scaffold initiated immediately leaving space for bone regeneration. HA development was confirmed by SEM/EDX analysis, X-ray diffraction, Raman and infrared spectroscopy after 5, 9 and 14 days (Figure 2). Ultra-violet visible and photoluminescence spectroscopies were used to evaluate the properties of the carbon dots and monitor the PLA degradation and HA development as well. Results indicate that this is a promising technique for confronting asymmetric or irregular-shaped bone fractures with simultaneous monitoring of the healing process.

Keywords: carbon dots, poly-lactic acid, 3D printing, bioactive scaffolds, bioglass® 45S5, bone regeneration, bioimaging.

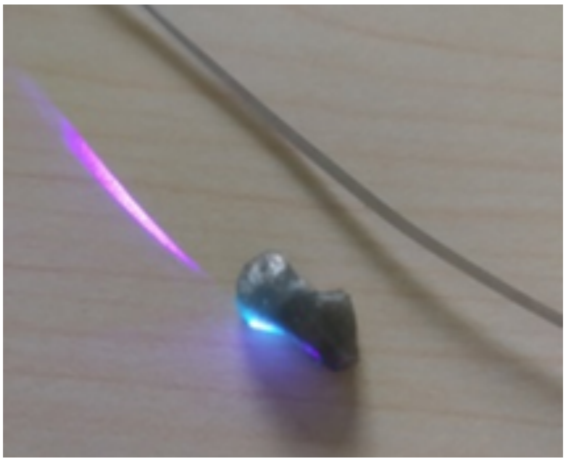

Figure 1: Fluorescence of a 3D-printed wrist scaphoid bone analog bioactive scaffold.

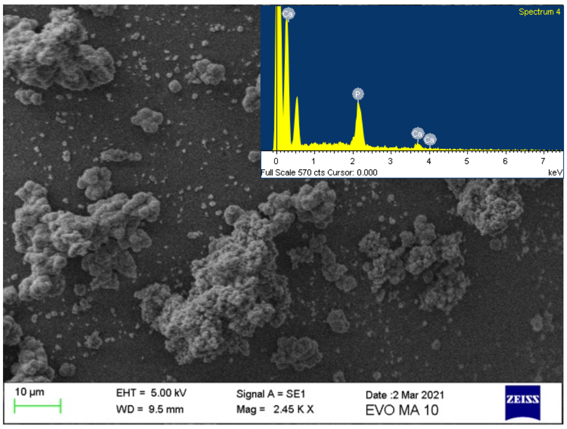

Figure 2: SEM image and EDX analysis of HA on a bioactive scaffold.

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Titanium Dioxide Multiscale Model for Simulation of Bio-nano Interfaces

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Abstract:

TiO_2-based nanomaterials are ubiquitous in important technological applications, yet their toxicological properties are uncertain[1, 2]. Modeling interactions of nanomaterials and biomolecules, such as membrane phospholipids, may help predicting nanotoxicity pathways. However, there is no practical way to model such interactions for sufficiently large nanoparticles with a representative fraction of the cell membrane if one uses an atomistic model. Thus, a more efficient and reliable model is required[3]. In this work, we develop a coarse-grained model of TiO_2-lipid systems (Figure 1) using structural data from atomistic molecular dynamics simulations with the inverse Monte Carlo method[4] implemented in the MagiC software package[5]. Molecular dynamics simulations are carried out using the GROMACS 2019 software package[6].

The atomistic simulations have revealed that DMPC and POPE phospholipids can adsorb on different anatase and rutile surfaces through the polar headgroups. Several different binding modes with varying adsorption strength have been identified. The resulting atomistic trajectories are mapped to the coarse-grained coordinates. During the coarse-grained bead mapping, the phospholipid molecules are reduced from ~100 atoms to ~10 coarse-grained sites, and the two surface layers of the TiO_2 slabs are reduced to the beads containing 5-7 atoms. Water molecules and the bulk TiO_2 are accounted for implicitly in the TiO_2-lipid effective potentials. Preliminary data show that the structural features of the TiO_2-lipid interface are well-reproduced in our coarse-grained model. However, the diffusion in the system is ~20 times faster due to the absence of water molecules.

This work has been supported by the EU Horizon 2020 research project SmartNanoTox (No 686098) and the Swedish Research Council. We acknowledge the Swedish National Infrastructure for Computing (SNIC) for granting access to high-performance computing facilities.

Keywords: nanotoxicity, TiO_2, bio-nano interface, lipid bilayers, multiscale modelling, coarse-graining, molecular dynamics.

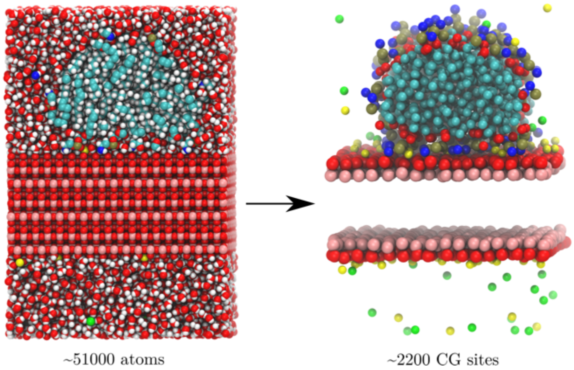

Figure 1: Snapshots of the simulated TiO_2-lipid system at the atomistic (left) and the coarse-grained levels (right). The image is generated using VMD[7].

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Detecting Hepatitis B Surface Antigen Using a Novel Polycrystalline Silicon Nanowire Biosensor

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Abstract:

The detection and monitoring of diseases are more and more important. Early detection and rapid analysis can effectively reduce the incidence of disease. Trace biomolecules detection using high-sensitive biosensors for disease diagnosis application is a potential and developing technology. The nanowire field effect transistor sensor has been proven to have many advantages such as high sensitivity, specificity, label-free and real time.[1] In this paper, a novel polycrystalline nanowire field-effect transistor (NWFET), which used a low-cost sidewall spacer etching technology to from the nanowire, was developed by our group to serve as a high-sensotivity biosensor. This polycrystalline NWFET sensor was used to detect Hepatitis B surface Antigen (HBsAg) proteins, which is one of biomarkers for screening infection of Hepatitis virus, to explore the stability and sensitivity of sensing components and make improvements.

The NWFET biosensors were fabricated on silicon wafers. The key process for the nanowire formation is that a TEOS oxide was deposited and patterned as a dummy gate, and then a polycrystalline silicon (poly-Si) film was deposited. The poly-Si film was etched back using a plasma etch system, as a result, a residue poly-Si line was left on the both sides of the TEOS oxide gate, as represented in Figure 1(a). The dimension of the Si nanowire depended on the etching parameter, and could be as small as 60 nm. This sidewall spacers technique could fabricated high-performance nanoscale silicon wires while avoiding expensive exposure system, thus significantly reducing production costs. The scanning electron microscope image of the poly-Si nanowires is shown in Figure 1(b).

Figure 2 illustrates the drain current (I_D) versus gate voltage (V_G) characteristics of the poly-Si nanowire FET biosensor at detecting HBsAg antigen of various concentrations. The black curve represents a baseline, that is, only buffer solution was on the sensor. The negative control sample using HBx antigen caused a slightly rightward shift (red curve). A more rightward shift was observed when HBsAg antigen was added to the sensor system, and the shift increased as the concentration of the target antigen is increasing. More data will be shown in the conference.

In conclusion, the poly-Si nanowire FET was successfully fabricated using a simle and cheap lithography and etch method, and was demonstrated to be a highly-sensitive biosensor for HBsAg detection. This novel biosnsor can be widely used in clinical applications in the future, as an early cancer screening or disease medical testing device.

Keywords: nanowire, SiNW, biosensor, hepatitis b surface antigen, HBsAg

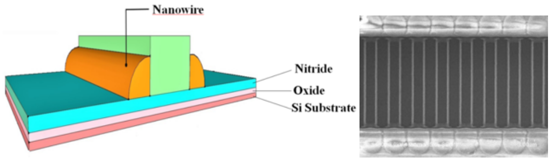

Figure 1. (a) Schematic representation of the nanowire formation using spacer etching technique. (b) Top-view scanning electron microscope image of the formed nanowires.

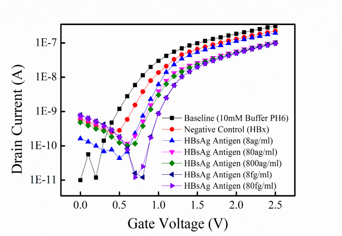

Figure 2. I_D-V_G curves of the SiNW FET biosensors in detecting HBsAg of different concentrations.

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Development of Nanozyme-based Sensors for the Detection of Reactive Oxygen Species

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Abstract:

Metallic nanoparticles such as gold nanoparticles (AuNP) have been shown to be able to catalyze specific reactions, similar to enzymes, herewith being classified as nanozymes. Their good conductivity, enhanced surface area and biocompatibility makes them excellent candidates for the development of label-free sensors as rapid screening tools for specific biomolecules, such as reactive oxygen species (ROS). An important ROS is hydrogen peroxide (H_2O_2). Through H_2O_2 detection, the antioxidant capacity of hydro-soluble plant extracts in food supplements can be analyzed and quantified [1].

We report the influence of biologically synthesized AuNPs on the sensitive and selective detection of H_2O_2. By reducing chlorauric acid ($HAuCl_4$) using various plant extracts, the AuNPs will have different functional groups, depending on the biomolecules present in the plant extracts: proteins, sugars, enzymes, amino acids and other metal traces. Thus, this work compares and highlights how biologically synthesized AuNPs lead to the development of label-free nanozyme-based sensor for rapid, sensitive and selective detection of H_2O_2 (Figure 1). Comparison will be made also with commercially available, AuNPs modified screen printed electrodes [2].

Electrochemical impedance spectroscopy (EIS), microscopy and UV-Vis spectrophotometry were used to monitor and characterize the biologically synthesized AuNPs. Analytical performances were evaluated by differential pulse voltammetry (DPV) and fixed potential amperometry, where high sensitivities and low detection limits were obtained.

Keywords: gold nanoparticles, biological synthesis, nanozyme based sensors, selectivity, specificity.

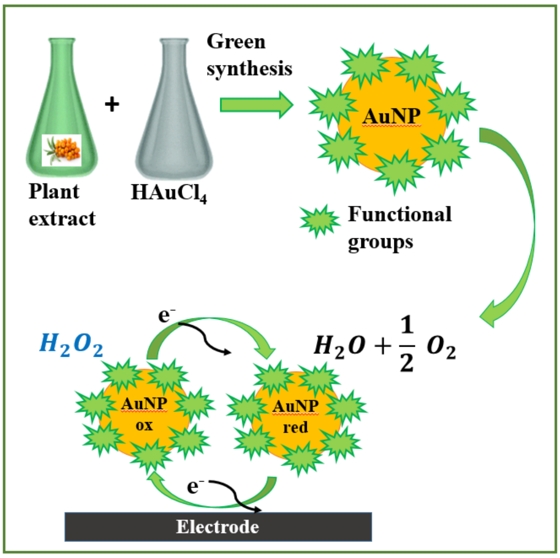

Figure 1: Figure illustrating the biological synthesis of AuNPs and oxidation mechanism of H_2O_2 catalyzed by biologically synthesized-AuNPs.

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Acknowledgments:

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Detection of non-conductive nanoparticles using Nanoparticles Imprinted Matrices (NAIMs)

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Abstract:

In the last decade, nanoparticles (NPs) have been in the focus of considerable cutting-edge interdisciplinary research. Nanotoxicology is a field that deals with the toxicity of NPs. As a result of this growing demand for NPs in research and industry, questions have been raised about their toxicity. The latter depends on their size, shape and the stabilizing shell. Therefore, there is an urgent need for new methods for specific recognition of NPs. The selective recognition of nanoparticles (NPs) can be achieved using nanoparticles imprinted matrices (NAIMs). In the NAIM approach NPs are imprinted in a matrix followed by their removal to form cavities that can reuptake the original NPs. The recognition of NPs by the matrix depends on supramolecular interactions between the matrix and the shell of the NPs, as well as on the geometrical suitability of the NPs to fit into the imprinted cavity. Thus far the NAIMs approach was limited to conducting NPs, specifically to metallic NPs. Herein, the NAIMs approach was expended to enable the detection of non-conductive NPs. Specifically, silica NPs were imprinted using electro-polymerization of aniline or phenol. The silica NPs were removed by dissolution with diluted HF solution. Latex NPs were deposited on an interdigitate electrode array (IDE) followed by spin-coating of sol-gel on the IDE-Latex-NPs to form the matrix. The latex NPs were removed by heating. The recognition of the NAIM system was determined by reuptake of the original or different NPs by the imprinted cavities using cyclic voltammetry or capacitance change.

Keywords: nanoparticles, nanotoxicology, imprinting, electrochemistry.

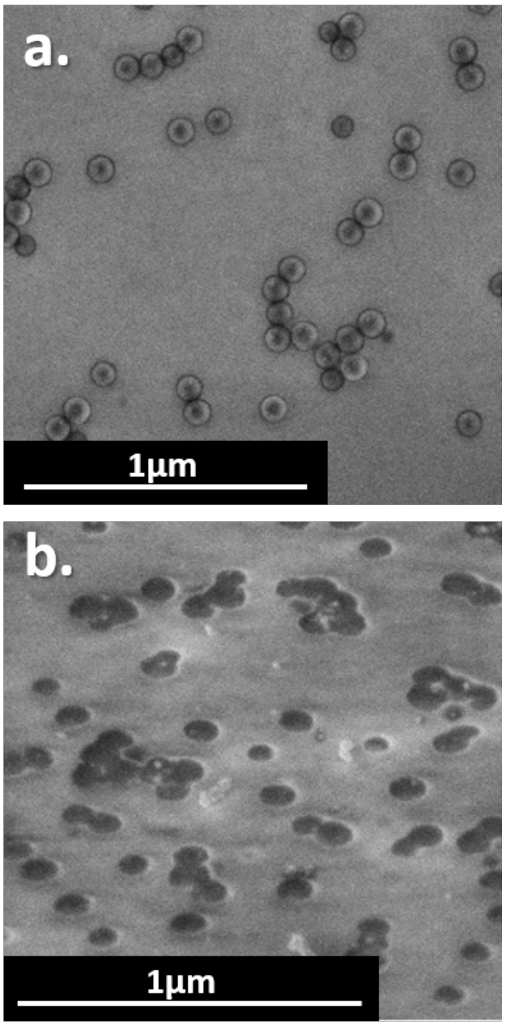

Figure 1: a). 100 nm Latex-NPs after spin coting of sol-gel matrix. b). Nano-cavities (100 nm) that were formed after removal of latex NPs.

Modification of Magnetite Nanoparticles with Triazine-Based Dendrons and their Application as Drug-Transporting Systems

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Abstract:
Dendrimers, which belong to a class of branched, homogenous, and polyfunctional macromolecules, have gained recently a significant attention due to their versatility of applications. Among the class of dendritic molecules, triazine-based dendrimers can be distinguished, which are built of triazine rings interconnected via nucleophilic linkers containing two or more either amine, hydroxyl, or thiol groups. Owing to several internal cavities between subsequent dendritic branches and numerous external free $-NH_2$, $-OH$, or $-SH$ groups, the macromolecules might exhibit various analytical, chemical, catalytic, or biomedical applications, in their native forms or immobilized on a support, which leads to the obtaining of hybrid materials [1]. The most commonly synthesized hybrid materials are inorganic-organic ones, containing chemically and physically stable, but also easily modifiable platforms, such as silica, titania, magnetite nanoparticles, or carbon nanotubes.

Herein, we present the synthesis of superparamagnetic Fe_3O_4 nanoparticles functionalized with triazine dendrons as convenient adsorbents dedicated to bioactive molecules' delivery. The choice of magnetite nanoparticles as support was undoubtedly driven by the easiness of a synthetic protocol leading to nano-sized particles, and the magnetic activity, which allows for their concentrating and/or separation using an external magnetic field. Encapsulation of Fe_3O_4 nanoparticles within a silica thin layer not only prevents the formation of magnetite aggregates but also facilitates surface modification through the incorporation of a wide range of silyl-derivatives into a silica matrix.

The obtained Fe_3O_4/SiO_2 systems were subsequently functionalized with triazine dendrons using a 'grafting from' approach based on a repetitive conjugation of cyanuric chloride and a particular nucleophile (e.g. piperazine, diethylenetriamine, or ethanodithiol). The obtained hybrid materials were examined for their adsorptive properties towards chosen drugs. The material-drug complexes were also tested for *in vitro* drug release in various media, affording paraphysiological conditions. The study proves the binding efficiency of magnetite-based hybrid materials modified with triazine-dendrons, but also shows how the use of particular interconnecting nucleophiles influences the ability of the materials to adsorb the chosen biocompounds. Due to the structure of dendrons, the presented materials may also find further application in water contaminants removal, pre-concentration of analytes facilitating trace analysis, or multiple catalytic reactions owing to the possibility of metal ions or metal nanoparticles entrapment within internal cavities.

Keywords: hybrid materials, triazine-based dendrons, magnetite nanoparticles, adsorption, drug transport; *in vitro* drug release.

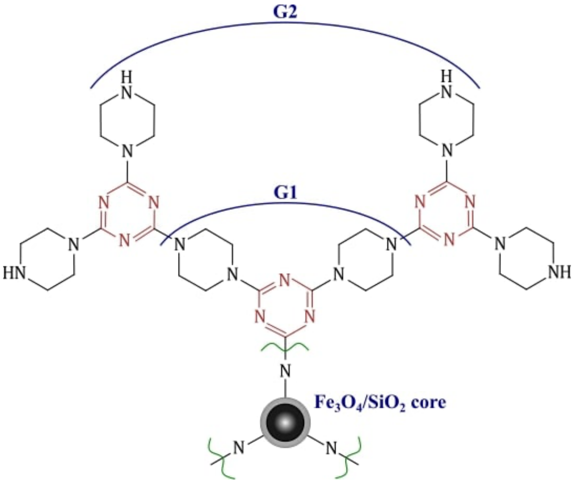

Figure 1: An exemplary Fe_3O_4-based nanomaterial grafted with piperazine-triazine dendrons; G1 and G2 correspond to generations of the synthesized dendrons.

This work was supported by grant no. POWR.03.02.00-00-I026/16 co-financed by the European Union through the European Social Fund under the Operational Program Knowledge Education Development.

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

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Abstract:

The development of cost-competitive materials capable of producing fuels or electricity directly from the energy harvested from sunlight offers a desirable approach towards fulfilling the need of clean energy. Recently, bismuth vanadate based photoanodes have attracted great amount of interest especially because of its narrow band gap energy between 2.4-2.5 eV, low cost and good stability. $BiVO_4$ is an n-type semiconductor and its use for solar water oxidation was first reported by Kudo et al. [1]. Nevertheless, $BiVO_4$ is disadvantages by its poor photogenerated charge carrier transport which leads to lower photocurrent density. We assembled CdS with $BiVO_4$ in order to obtain heterojunction formation and hence to achieve an even better photoelectrochemical response. However, the CdS suffers from photo-unstability which is its main drawback during the photo-illumination measurements. Then, CoO_x was loaded on the surface of CdS in order to improve both, PEC performance and stability [2]. The surface morphology images (Figure 1) were examined by Scanning Electron Microscope (SEM) and High Resolution Transmission Electron Microscope (HR-TEM). Observed from the SEM images BiOI are formed by very thin 2D plate-like nanosheets attached vertically to the FTO substrate which are after chemical and thermal treatment converted to round particles of $BiVO_4$. Fig. 1c demonstrates successful synthesis of $BiVO_4$/CdS heterostructure. The EDS elemental mapping reveals that CdS was homogeneously deposited on the surface of $BiVO_4$ while the CoO_x was randomly dispersed on the top that is usual for metal oxides serve as co-catalysts. To confirm the potential usage of the samples as photoanodes, the linear sweep voltammograms were measured. The current densities generated on bare $BiVO_4$ and CdS are 2.1 mA cm^{-2} and 1.9 mA cm^{-2}, respectively. Among them, current density of 4.54 mA cm^{-2} was obtained for $BiVO_4$/CdS which is more than two times higher than that of blank counterparts.

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

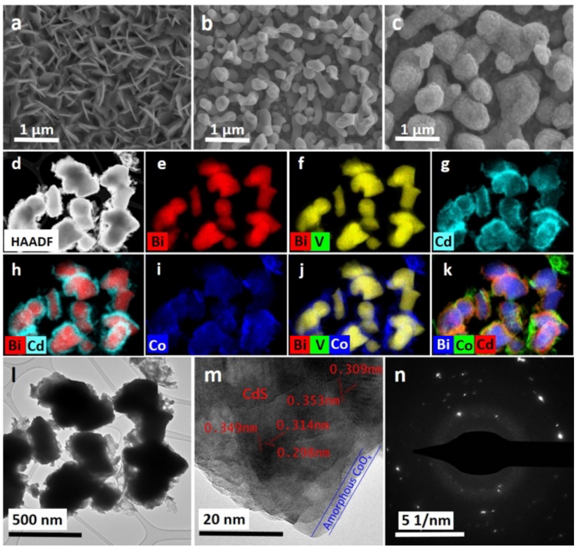

Figure 1: SEM images of (a) BiOI; (b) $BiVO_4$; (c) $BiVO_4$/CdS composite; (d) High-angle annular dark field (HAADF) image and (e-k) EDS elemental mapping of Bi, V, Cd, Co, joined Bi-V-Co and Bi-Co-Cd taken from $BiVO_4$/CdS/CoO_x composite; (l, m) HR-TEM images and (n) selected area electron diffraction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

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Development of an AFM-based technique for extended write/erase endurance measurements of memristive cells

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Abstract:

Memristors are devices composed of materials whose electrical resistivity can be modified by application of adequate bias voltages. The resistance state of {electrode/film/electrode} memristive cells may thus be reversibly switched between at least two regimes: a high-resistance state R_{High} and a low resistance state R_{Low}. Switching repeatedly between R_{High} and R_{Low} allows to obtain the maximum number of "write/erase" cycles before failure. Such parameter (denoted endurance) is interesting to examine [1,2] towards potential applicabilities to non volatile memories or bio-inspired neuromorphic circuits.

Usually, wires and/or macroscopic probes are used to apply a bias between the electrodes of the studied cell, provided the electrodes are large enough (≥ 100x100 µm²). If these electrodes are too small or fragile, they need to be electrically connected to intermediate remote larger areas which are wired to the measurement unit.

Here, we report a simple endurance measurement technique based on Atomic Force Microscopy (AFM): a small AFM conducting probe (tip radius < 30nm) touches directly the top electrode of the cell. In this configuration, application of pulses and measurements of resistance states can now be carried out in a completely automated way, either in ambient air, or under lower relative humidity (RH ≤ 2%). Such a technique has been applied to {Au/Li_xCoO_2/doped Si} memristive cells (Figure 1).

Keywords: resistive switching, Atomic Force Microscopy (AFM), non volatile resistive memories (ReRAM), write/erase cycles, endurance.

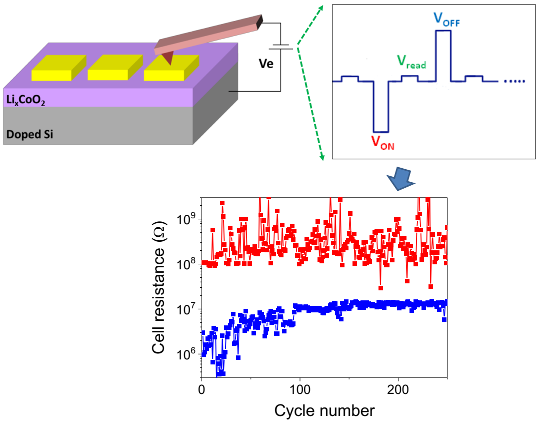

Figure 1: Top-Left: schematic view of the set-up. Top-Right: shape of the voltage pulses applied. Bottom: evolution of R_{High} (red) and R_{Low} (blue) of a 100x100 µm² {Au/Li_xCoO_2/doped Si} cell, under dry air (RH ≤ 2%, read voltage: 0.1V).

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Structural and dielectric properties of $CoFe_2O_4 \backslash LiNbO_3$ Bilayers

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Abstract:

Nanostructured multiferroic thin films constructed by combining magnetostrictive and piezoelectric materials have attracted recently much scientific and technological interest [1,2]. In addition to possessing ferroelectricity and ferromagnetism in each phase, they are shown to exhibit stress-mediated coupling between their magnetic and electric properties, called the magnetoelectric effect. This coupling between their magnetic and electric degrees of freedom may then give rise to new physical phenomena and applications.

Lithium niobate ($LiNbO_3$) is a ferroelectric material with good piezoelectric, pyroelectric, electro-optical, birefringent, photorefractive and photoelastic properties which are favorable towards applications. Cobalt ferrite ($CoFe_2O_4$) presents a high magnetocrystalline anisotropy and magnetostriction, making it suitable for application in magnetoelectric composite thin films.

Here, bilayer composite thin films, composed by a $LiNbO_3$ layer deposited over a $CoFe_2O_4$ film have been prepared by laser ablation on platinum covered Si(001) substrates. Their structural, microstructural and dielectric properties were characterized. The X-ray diffraction measurements show a rhombohedral ferroelectric phase in $LiNbO_3$ and a cubic spinel structure in $CoFe_2O_4$. The SEM micrographs show dense films, with cobalt ferrite and lithium niobate layer thicknesses in the range 100-200nm and 300-800nm, respectively. Their dielectric properties were characterized by impedance spectroscopy. To obtain the relaxation times and activation energies, the electrical permittivity (figure 1) was fitted, using appropriate models for the behavior of the polarization and including a conductivity contribution. As such, the influence of the synthesis conditions on the dielectric properties of the films and their evolution with individual layer thicknesses will be discussed.

Keywords: Cobalt Ferrite, Lithium Niobate, Multiferroic composites, Thin films, Laser Ablation, Structural properties, Morphology, Dielectric properties, Impedance spectroscopy.

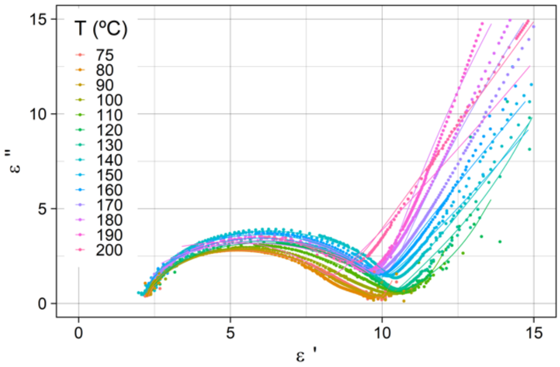

Figure 1: Nyquist plot, with the imaginary component of the electrical permittivity as a function of the real component, for a film with a layer of $CoFe_2O_4$ with a thickness of 152nm and 376nm for the $LiNbO_3$.

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Flexible and Large-area Electrochromic Films based on PEDOT:PSS for Smart Windows

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Abstract:

Electrochromic devices have attracted extensive attention in the recent decades. Electrochromism is the phenomenon which change their optical absorption when ions are inserted or extracted via a centrally positioned electrolyte. In recent years, with popularizing energy-efficient systems and green buildings, smart window using electrochromic devices have attracted a lot of attention in the decades. A typical electrochromic device is composed of transparent conductors, electrochromic films, and electrolyte. Fluorine doped Tin Oxide(FTO) and Indium Tin Oxide(ITO) glass, which are mostly used as the transparent conductor, do not meet the requirement for flexibility. ITO films, which were grown at low temperature by sputtering on PET substrate, also need a long-term improvement in durability by bending test. To respond to these drawbacks, numerous organic materials including graphene, carbon nanotubes, and conducting polymers are being actively investigated as a replacement for ITO. Among the alternatives, poly(3,4ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) have been reported to exhibit excellent flexibility and show high electrical conductivity, optical transparency on repeated bending cycles. Recently, the reported electrical conductivity range of PEDOT:PSS is about 2000~4000 S/cm by various film and solution treatments. PEDOT:PSS is also promising electrochromic materials as well as metal oxides (e.g. WO_3, TiO_2, NiO_X, V_2O_5, etc.). Hence, PEDOT:PSS electrochromic devices can have a simplified configuration that simultaneously play the transparent conductor and the electrochromic layer role. In this works, we repot a flexible and ITO-free electrochromic(EC) film based on PEDOT:PSS with high optical contrast and simple configuration. In fact, PEDOT:PSS EC film have only three layers, PEDOT:PSS(working, counter electrodes) and polymer electrolyte layer cured by ultra violet(UV) light. These devices were tested for electrochemical cyclic stability and mechanical bending test and large-area EC films with size of 250mm x 2,000mm (width x length) were fabricated by Roll-to-Roll wet coating process.

Keywords: Smart window, Electrochromic film, conducting polymer, PEDOT:PSS

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Overheating on aluminum metafilms by non-radiative decay of surface plasmons

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Abstract:

In the last few years the study of the surface plasmons (SP), results to be relevant in the research of the generation of hot electrons[1] that transfer their energy to the phonons, thus increasing temperature (T) locally[2].

In the present work, we studied the increase in T of systems formed by thin aluminum (Al) films deposited on texturized substrates of Porous Anodic Alumina (PAA) obtained by electrochemical anodization of Al foils. We denominated these systems aluminum metafilms (Al-MF) as shown in Figure 1-a).

During the anodization process we can vary the geometric parameters such as the interdome distance (D_I) (Figure 1-a)) of the Al-MF, by this way in the reflectance measurements, we observe dips associated with surface plasmonic resonances (SPR) at determined wavelengths that are a D_I function[3] shown in Figure 1-b.

The measurements of T as a function of the intensity of incident radiation, showed T increases up to ~200 K, these attributed to Al-MF morphology and hot electrons result of the non-irradiative decay of the SP (Figure 1-c)). Locally, the temperatures reached due to non-radiative decay of SP are estimated to be ~933 K (melting point of Al).

On the other hand, due to local heating in Al-MF, measuring the electrical resistivity (ρ) as a function of the radiation exposure time (t_{exp}) it was observed that when the Al-MF were irradiated, as a result, ρ began to increase. When the t_{exp} were greater than ~4 s, irreversible changes in morphology (Figure 1-d) and change in the slope of ρ (Figure 1-e), due to degradation and subsequent evaporation of Al from the samples were also observed.

Keywords: aluminum, surface plasmons, metamaterials, hot carriers.

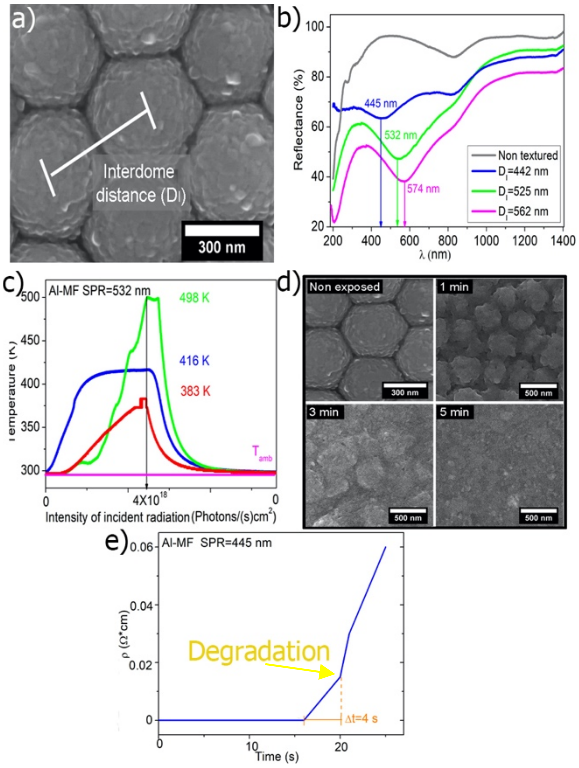

Figure 1: Figure 1: a) SEM image of Al-MF (D_I depends on the applied voltage in the anodizing process). b) Reflectance spectra of Al-MF with different D_I. The results of the non-texturized Al film (gray curve) are shown for comparison. c) T curves as a function of the incident radiation in Al-MF with SPR=532 nm illuminated with wavelengths=445 nm (blue), 532 nm (green) and 650 nm (red). d) SEM images from the morphology evolution of an Al-MF irradiated at the different $t_{exp.}$ e) ρ curve of Al-MF with SPR=445 nm irradiated with wavelength=445 nm.

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Numerical Study of Graphene Oxide Capacitive Humidity Sensor with Novel Etching Configuration

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Abstract:
Capacitive humidity sensors have aroused tremendous interest due to their vital use in agriculture, electronics, semiconductor processing, medical monitoring, etc. There is a huge interest in developing high sensitivity, high stability, high reproducibility, and fast response and recovery time sensors to instantly provide a reliable and accurate reading of the humidity levels in the surrounding environment. Graphene oxide, an oxidized form of graphene, is a promising candidate as a sensing material in humidity sensors due to its hydrophilic oxygen-containing functional groups [1]. Here, we report a numerical study of graphene oxide humidity sensors using COMSOL Multiphysics®, focusing on the effect of geometric dimensions. The configuration of the humidity sensor comprises of graphene oxide sensing film sandwiched between lower and upper parallel electrodes. Firstly, a systematic study on configurations was performed by altering different parameters, such as the electrode width and spacing, sensing material thickness, and overall dimensions of the device with a comparison and analysis on response time and sensitivity. In addition to typical configurations, we also evaluated the trench effect on the sensitive layer in humidity sensors, which can be fabricated using the etching process found in cleanroom technology. Our preliminary simulation results indicated that a configuration with the etched profile shows a better sensing performance, with a 67% improvement in response time, as indicated by Fig. 1. This study can be used as a parametric relationship reference when designing humidity sensors. Moreover, the proposed etched novel structure has the potential to further enhance sensor performance in the semiconductor industry.

Keywords: Graphene oxide, capacitive humidity sensor, parallel plate humidity sensor, isotropic etching.

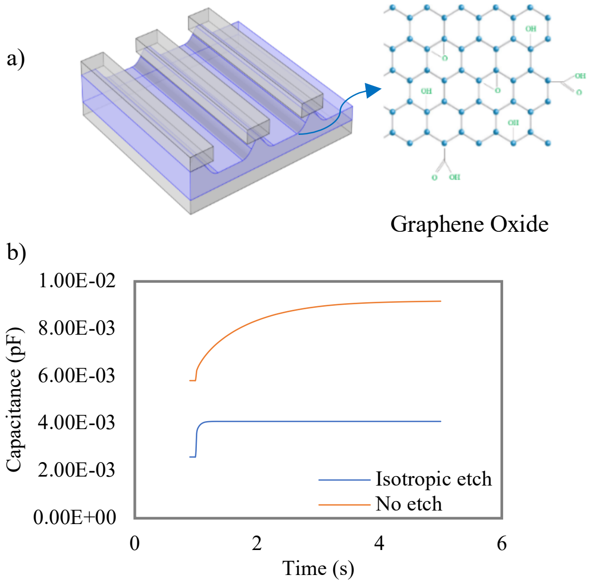

Figure 1: a) The modelled capacitive humidity sensor consisting of graphene oxide as the sensing material sandwiched between the lower and upper silver electrodes with a novel isotropic etched profile. b) Response time comparison of the etch and non-etch profile configurations of the sensor subjected to relative humidity of 90% at 25°C.

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Design of visible-light photocatalysts for NOx removal based on LDH/BiOX nanolayered heterojunction

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Abstract:

Over the previous years it has been demonstrated that a single semiconductor-based photocatalyst cannot satisfy all the requirements to achieve high photocatalytic efficiency, as a complete solar light harvesting, a suitable energy band locations for redox reactions, greater photostability and efficient charge carriers separation. In this sense, the present study proposes the construction of new electronic structures by coupling inorganic semiconductors to enhance their practical application for the photocatalyic removal of NOx gases from polluted air. In that way, we considered that Layered Double Hydroxides (LDH) and Bismuth Oxyhalides (BiOX, X=Cl, Br, I) (Figure 1) could be a suitable pair because of their inherent structural flexibilities and a favorable photocatalytic capacity under visible-light irradiation, respectively [1,2]. BiOX compounds were obtained via co-precipitation method and MgAl-LDH compounds were prepared using a new synthesis strategy known as the AMOST method (*Aqueous Miscible Organic Solvent Treatment*), described by O'Hare et al. [3]. Through this method highly dispersed porous solids exhibiting highly surface areas and low powder densities are obtained. The adequate preparation of BiOX/MgAl-LDH systems will be carried out by homogeneous mixing in liquid medium using the *BÜCHI mini Spray Dryer B-290* equipment and a full caractherization will be done in order to know the properties of this new semiconductor. Preliminary results concerning to the characterization of the semiconductor heterostructures and their photocatalytic properties were studied.

Keywords: LDH; BiOX; Heterojunction; Advanced Photocatalyst; Nitrogen oxide

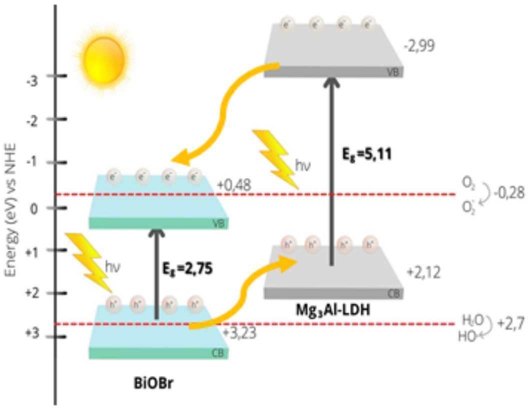

Figure 1: Schematic diagram of charge transfer occurring in LDH/BiOX heterojunction under visible-light irradiation.

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Hydrotalcite-like material for a double environmental remediation

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Abstract:

Layered double hydroxides (LDH) are a group of anionic clays that have found several practical applications. These materials have been widely studied as a sorbent of the wastewaters pollutants. Chromium (VI) is one of the most dangerous contaminants which reach natural waters as an effluent of different industries such as leather, textile or metallurgy. This specie can be removed from the contaminated waters by using layered doubles hydroxides as a sorbent. However, the regeneration of the sorbent is an expensive procedure [1]. So in this context, we report the revalorization of this used sorbent as a photocatalyst for environmental remediation [2] (Figure 1). Magnesium-Aluminium layered double hydroxides synthesized by coprecipitation method have been studied for the elimination of NO_x gases, before and after its use as a chromate sorbent. A complete chemical, morphological, photoelectric and photochemical study of the samples was carried out. Results showed that LDH materials presented no significant changes in their structure after their use as a sorbent. Photocatalytic tests of the samples showed a very good NO removal efficiency, as well as a high selectivity (no NO_2 emissions) through complete oxidation of these oxides to nitrate. The incorporation of chromate into the LDH structure improved the absorption of light in the visible region of the spectra, producing an improvement of 18% in the NO elimination compared with the LDH without chromate.

Keywords: layered doble hydroxide, chromate, photocatalyst, environmental remediation, NO_x, wastewater.

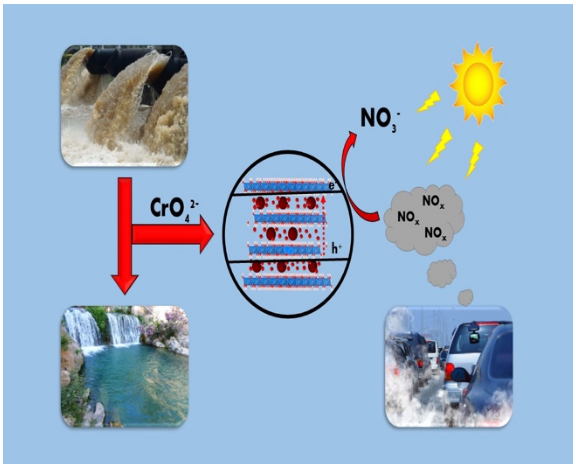

Figure 1: Figure illustrating the revalorization of the LDH sorbent with chromate as a photocatalyst for the removal of NO_x gases produced by combustion of fossil fuels.

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Challenges on the investigation of Fluorecent Probes for Heavy Metal-based Nanomaterials

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Abstract:

The extended release into the environment of heavy metal-based nanomaterials, in combination with their adverse effect on aquatic life, raises the demand for reliable and affordable techniques for their detection[1]. Among analytical methods, which can be useful for detecting nanomaterials in watery samples[2], fluorescence-based sensing remains one of the most promising approaches due to its simple solution assay processing, low cost, rapid response and high sensitivity, as well as its high selectivity through molecular binding design. With the aim of investigating the development of an easily synthesized dansyl-based fluorescent probe for detecting heavy metal-based nanomaterials in aqueous solution, with short response time, we have designed a Schiff base ligand H_2L (Figure 1). This derives from the reaction of 4-formyl-3-hydroxybenzoic acid with N-(2-aminobenzyl)-5-(dimethylamino)naphthalene-1-sulfonamide.

H_2L incorporates a suitable O,N-binding domain that can bind heavy metal ions as Cd^{2+}. Therefore, H_2L is suitable to interact with Cd^{2+} at the surface of the particles giving inner sphere complexes by ligand exchange[3]. Changes in fluorescence emission spectra of H_2L upon titration with non-fluorescent CdSe nanopowder have been investigated at neutral and basic pH. Figure 1 shows the fluorescence spectrum of H_2L before and after the addition of the same amount of CdSe nanopowder. It mus be noted that deprotonation of H_2L at basic pH not only favors formation of the inner sphere complex, but also results in an enhancement of the fluorescence intensity, which is accompanied by a blue-shifted of λ_{em}. It is clear that regardless of pH the addition of CdSe nanopowder results in quenching of the fluorescence. However, at basic pH quenching is more pronounced (about 75%) and it is accompanied by a clear blue-shifted of λ_{em} (hypsochromic shift). Therefore, there are enoughtly strong evidences that encourage us to continue investigating this topic.

Keywords: CdSe nanopowder, fluorescent probes, fluorescence spectroscopy, UV-Vis spectroscopy, inner sphere complexes.

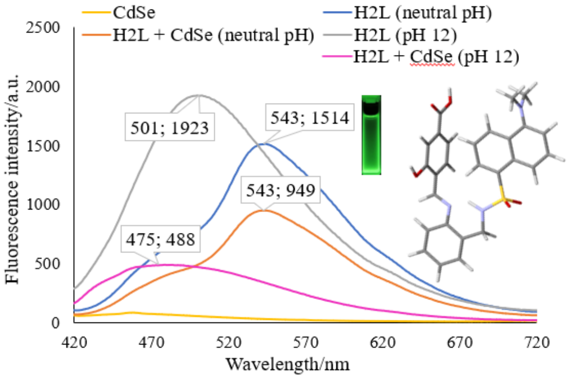

Figure 1: Figure illustrating the fluorescence spectra of H_2L before and after interaction with CdSe nanopowder at neutral and basic pH.

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Metallic Nanocatalysts for Glycerol Valorization

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Abstract:

Glycerol is the main by-product in transesterification-based biodiesel manufacturing, where 100 tons of biodiesel produced yields ~ 10 tons of crude glycerol. Expansion of global biodiesel production has led to glycerol excess on the market, resulting in a significant price drop.[1] Conversion of surplus glycerol to more valuable compounds can help with the problem. Glycerol electrooxidation reaction (GEOR) is a complex process during which a number of commercially viable intermediates and compounds are generated on the anode. These include chemicals like oxalic acid (OA), tartronic acid (TA), hydroxypyruvic acid (HYDP), dihydroxyacetone (DHA), glyceraldehyde (GALD), and glyceric acid (GA), which are up to 1000 times more expensive than crude glycerol. Moreover, such an approach has additional advantages—reduced manufacturing costs for the value-added chemicals and the co-generation of hydrogen on the cathode. One of the most promising approaches is electrocatalytic oxidation utilizing metallic nanoparticles. For example, platinum-based nanostructures have been widely studied as a catalyst for the GEOR because of the high activity and excellent stability of Pt in acidic and alkaline media. Furthermore, it has been reported that bimetallic catalysts outperform pure platinum and, by varying composition, shape and size of the nanocatalysts, selective formation of the products can be accomplished.[1–3] Additionally, GEOR selectivity can be tuned by different crystallographic facets involved in the catalysis.[4]

In the present study, we have investigated octahedral (Octa) Pt and Pt_xNi_y nanocrystals enclosed by {111} facets, as catalysts for the GEOR in alkaline media. The materials were synthesized via a solvothermal method.[5] The morphology and composition were confirmed using SEM-EDS, HRTEM, and EDX. Influence of the ratio of the metals on the catalytic activity and selectivity was investigated, as well as temperature and electrolysis time. Chronoamperometric measurements for PtNi at 25°C and 60°C have shown that the selectivity of GA and TA formation is up to 60% and 16%, respectively. Additionally, product concentrations were almost doubled at the higher temperature. For the $PtNi_2$ catalyst the GA selectivity was found to be 70% at both 25°C and 60°C. Concentrations of GEOR products were determined via HPLC at 30°C with a two-column setup and refractive index detector.

Keywords: glycerol electrooxidation reaction, value-added products, selectivity, platinum, PtNi nanoparticles

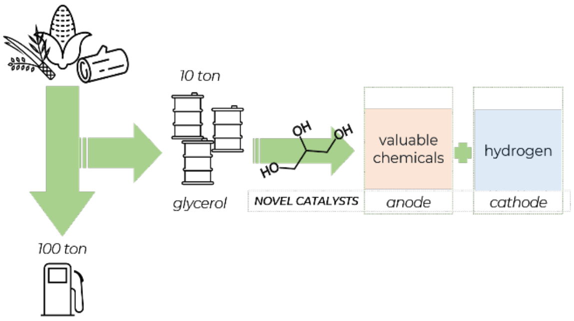

Figure 1: A sustainable approach to glycerol valorization.

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A Comprehensive *In Vivo* Study Using *Drosophila melanogaster*: New Insights into Mechanisms and Biological Effects of Permethrin Nanopesticides

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Abstract:

Understanding the interaction between nanopesticides and edible plants is crucial in evaluating the potential impact of nanotechnology on the environment, human health, animal health, and agriculture. While *in vitro* testing offers some potential, *in vivo* research into toxic effects of permethrin and permethrin nanopesticides could yield much more reliable data. *Drosophila melanogaster* has recently gained significant popularity as a dynamic eukaryotic model in examining toxicity, genotoxicity and biological effects of exposure to nanomaterials, including viability, morphological deformations, locomotor activity, phenotypic variations, internalization, lipid peroxidation product formation (malondialdehyde), oxidative stress (glutathione (GSH) content), intracellular reactive oxygen species production, and genotoxicity [somatic mutation and recombination test (SMART) and Comet assay]. We employed *D. melanogaster* as a model organism in our study to identify the potential risks of exposure to permethrin at concentrations ranging from 0.01 to 0.1 mM and permethrin nanopesticides at concentrations ranging from 0.01 to 2.5 mM. Exposure to permethrin and permethrin nanopesticides at highest two concentrations produced significant morphological defects, impaired climbing behavior, and genotoxicity. This is the first study to report findings of nanogenotoxicity, phenotypic variations and locomotor behavior in *D. melanogaster*.

Keywords: *Drosophila melanogaster*, permethrin, nanopesticides, nanogenotoxicity, risk assessment

Acknowledgments

This research is supported by the Scientific and Technical Research Council of Turkey (TUBITAK) (Project ID: 119Z208), Ankara (Turkey).

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Interferometric Reflectance Imaging Sensor (IRIS) applied to the real-time binding detection of mycotoxin fumonisin B1

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Abstract:
Mycotoxins are secondary metabolites produced by microfungi (moulds). These naturally-produced compounds can be found in many food products, and they are extremely harmful for humans, causing disease (mycotoxicoses) which may lead to death [1]. With this premise, the ability to efficiently detect the presence of mycotoxins in food products clearly emerges as a critical issue in food industry, especially for food quality control. One of the features of these toxic molecules is their low molecular weight (<700Da), which renders the measurement of their binding kinetics quite challenging. Here, we demonstrate the small-molecule sensitivity of the Interferometric Reflectance Imaging Sensor (IRIS) [2] by achieving the label-free, real-time detection of fumonisin, a mycotoxin produced by Fusarium fungi species and diffusely found in corn and other agricultural products. Twenty antibodies that tested positive to fumonisin B1 in an ELISA assay were immobilized onto an active SiO_2/Si IRIS chip in a microarray modality. A solution of Fumonisin B1 was then flowed across the chip surface while real-time reflectance images were recorded. By measuring the slight increase in reflectance due to biomass accumulation, the dynamic binding of fumonisin to the immobilized antibodies was detected. 17 out of the 20 analyzed antibodies tested positive to fumonisin in our assay. The kinetic constants (k_{ON}, k_{OFF}, K_D) were calculated, allowing to fully characterize and classify the antibodies. The next steps will be to perform a similar characterization of the two other existing species of fumonisin (fumonisin B2 and B3), as well as a deeper investigation of the antibodies that yielded the best results in terms of kinetic constants, to finally determine which one would be the best for direct food quality control applications.

Keywords: Mycotoxins, Fumonisin, food toxins, label-free detection, biosensors, IRIS, binding kinetics, interferometric detection.

Figure 1: Fumonisin effect on a corn cob. The poor kernel structure is a consequence of the toxic action of the fungi (Jourdan Bell, Texas A&M AgriLife).

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Contribution to the knowledge of the Family Elateridae, Coleoptera from the Kingdom of Saudi Arabia

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Abstract

In the King Saud University Museum of Arthropod, Riyadh, approximately 3,000 specimens of the click beetle family Elateridae, collected throughout the Kingdom of Saudi Arabia, including economically important taxa are deposited. By using existing identification tools that rely solely on morphological characters and internal genitalia. However, it is well-known that many elaterid species previously described from Saudi Arabia are poorly or incompletely characterized morphologically, making identifications often problematic. DNA barcoding has been successfully implemented in numerous studies of beetles to assist in specific identification of previously described species, and often revealing cryptic species.so in this study use mitochondrial and nuclear DNA sequence data to delimit selected putative species using the genus *Cardiophorus* as an example. The DNA sequencing in this study occurs some genetic variation between tow genus *of Craspedostethus: C. flavescons* and *C. dilutes*, family Elateridae.

Keywords

The click beetle *Craspedostethus flavescons* and *C. dilutes*, DNA barcoding, Sequencing.

Multifunctional Nanocoatings to Overcome Contact Lenses Associated Conditions and Discomforts

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Abstract:

While contact-lenses possess voluminous beneficial applications for visual-correction, they are also the prime threat to the development of ophthalmic impediments, e.g., infiltrative keratitis, contact-lens acute red eye, contact-lens-induced peripheral ulcer, and microbial-keratitis. Eye-infections resulted from the microbial adulteration of lens care solution, lens cases, and contact-lens wares that are further intensified using unsanitary lens care and extended lens wear. The most common pathogenic microbes responsible for ocular infections are gram-positive bacteria, gram-negative bacteria, fungi, viruses, and amoeba. We have recently developed a multifunctional antimicrobial coating for contact lenses, adopting a single-step sonochemical approach using plant-mediated synthesized ZnO NAPs, Gallic acid, and antibacterial drug (Tobramycin). The contact lens coated with multifunctional antimicrobial coating was evaluated for its antioxidant activity and antimicrobial performance against different pathogenic microbes such as *S. aureus*, *E. coli*, *P. aeruginosa*, and *Candida albicans*. They are also evaluated for their biocompatibility. The formation of nanocoating on the contact lens has successfully been confirmed with different spectroscopic techniques, including XRD, EDX, SEM, FTIR. The coated contact lens significantly inhibited the growth of pathogenic microbes and presented excellent antibacterial and antifungal properties. They also demonstrated excellent antioxidant and biocompatibility performance. Multifunctional coatings containing plant-mediated synthesized ZnO NAPs, Gallic acid, and antibacterial drug (Tobramycin) were engineered on contact lens without altering their geometry and refractive properties through one step, fast, robust, and reproducible sonochemical process. Our current research work will open new directions for the functionalization of different medical devices, including contact lens, urinary, and vascular catheters, etc., with hybrid antibacterial coatings without modifying the properties of their bulk materials.

Keywords: Contact lens, nanocoating, bacteria, fungi, biocompatibility

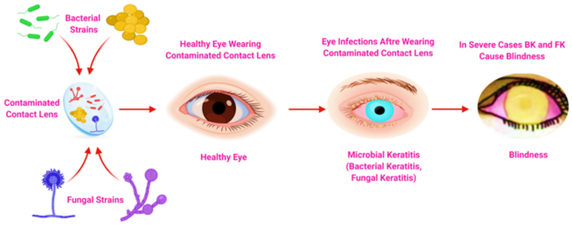

Figure 1: Eye-infections resulted from the microbial adulteration of lens care solution, lens cases, and contact-lens wares

References:

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Studies on the possibility of using modified titanium oxide as a potential drug carrier

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Abstract:
The impact of nanomaterials on the functioning of individual organs of living organisms clearly indicates the fact that that the use of nanoparticles as carriers of medicinal substances is associated with the negative effects of their accumulation in human and animal tissues. In the studies a series of stable nanocarriers based on titanium (IV) oxide nanoparticles, modified by introducing into their structure substances ensuring the reduction or elimination of their toxic properties has been obtained. In order to achieve the intended results, the nanoparticles have been formed in the presence of substances that when embedded in their structure may protect them against harmful activity. Carbohydrate coating on the surface of titanium dioxide nanoparticles can modulate the course of both oxidative stress and cellular uptake which can be the effect of releasing of titanium ions. The reducing of toxic properties is achieved by the addition of organic substance (galactose). This carbohydrate prevents the dissolution of titanium dioxide and thus limits the releasing of toxic titanium ions. The oxidative stress is mainly responsible for the toxicity effect. It was confirmed that nanoparticles covered with carbohydrate molecules were much less toxic to neuronal cells and hepatocytes compared to nanoparticles to which glucose (polysaccharide), citrate residues or ethylene glycol has been attached [1].

Modified titanium dioxide nanoparticles have been in the field of microwave radiation. The products were varied depending on the values of the process parameters such as process time and amounts of reagents (quantitative parameters). The products have been characterized by providing the size of nanoparticles, their specific surface, XRD diffractograms FTIR spectra and TEM microphotographies. Also, the analysis of titanium ions in different environments (waer, SBF and Ringer solutions) has been performed. It was found out that the releasing of titanium ions from the modified titanium dioxide nanoparticles is significaly reduced when comparing to pure TiO_2 powder.

This work is a part of the project "A method of producing non-toxic carriers of active substances based on nanomaterials," supported by the National Centre for Research and Development, Poland under the agreement LIDER/20/0080/L-9/17/NCBR/2018.

Keywords: drug carriers, titanium dioxide, nanomaterials, transport systems.

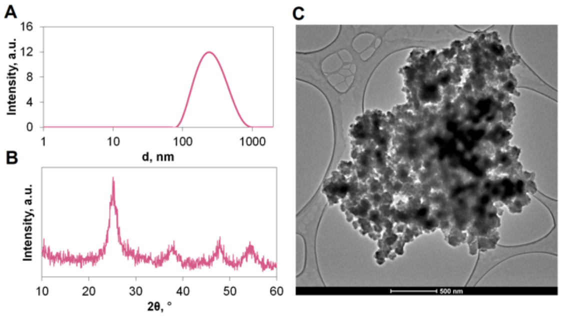

Figure 1: A) Particles size distribution, B) XRD diffractogram, C) TEM microphotography of TiO_2 nanoparticles modified with galactose.

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Efficient photodegradation of dye-polluted water by a high-flowrate functionalized microreactor

N. Martin[1,*], V. Lacour[2], C. Perrault[2], E. Roy[2] and Y. Leprince-Wang[1]

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Abstract:
With climate change and the increasing ecological pressure humans cause on the Earth water resources, it is necessary to find and develop efficient and environment-friendly water remediation processes, to ensure the good quality of the water resources available to Humanity. Photocatalysis has already proven its efficiency to degrade organic pollutants in water, using only a reusable photocatalyst and UV light[1]. Thus, the integration of photocalysts in microreactors to increase their efficiency is a crucial step in the development of new photocatalytic reactors for water purification. However, the flowrate (in mL/day) of such reactors is still an issue[2]. In this work, we used an innovative, optically transparent, and chemically stable polymer developed by Eden Tech[3], Flexdym™, to easily produce microreactors able to support high flowrates (more than 4 L/day), thanks to their original design. We then used an easy and low-cost hydrothermal synthesis method to continuously grow ZnO nanowires *in situ*, while studying the impact of the growth temperature, time and flowrate on the morphology and the photocatalytic efficiency of the samples, by degrading continuous flows of Acid Red 14 (AR 14) at 10 µM/L under UV light. We demonstrated that, in the optimal synthesis conditions with a growth flowrate of 200 µL/min, a growth time of 1h and a growth temperature of 80°C, our microreactors can degrade between 82% and 98% of AR 14 in a time equivalent to 40s under UV light at a photocatalysis flowrate of 200 µL/min (Figure 1), and 87% in 20s at 500 µL/min (not shown here).

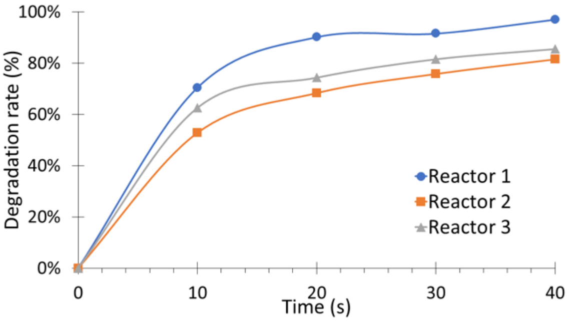

Figure 1: Mean photodegradation of AR 14 by three of our functionalized-high-flowrate microreactor under UV light.

Keywords: ZnO nanowires, Photocatalysis, Microreactors, Hydrothermal growth, Dye degradation

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Supercritical Fluid Extraction and Pressurized Liquid Extraction Processes Applied to EPA-rich Polar Lipid Recovery from the Microalga *Nannochloropsis* sp.

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Abstract:

This work studies the simultaneous extraction and fractionation of saponifiable lipids (SLs) into neutral saponifiable lipids (NSLs) and polar lipids (phospholipids, PLs, and glycolipids, GLs) from the microalga *Nannochloropsis* sp. (41.9% NSLs, 58.1% polar lipids, 32.5% EPA) to obtain EPA-rich polar lipid fractions, using green techniques (Figure 1). Several two-step extraction processes were studied, combining CO_2 supercritical fluid extraction (CO_2 SFE), pressurized lipid extraction (PLE), and ethanol-gas (CO_2) expanded extraction (ethanol-GXE). Extraction at atmospheric pressure, including the Soxhlet extraction method, was used as the reference. Firstly, a lipidic fraction rich in NSLs (80.4% of total SLs), was obtained using hexane and the Soxhlet extraction method; this extract contained 85.8% of the biomass NSLs. Subsequently, in the second extraction step using ethanol (96%), an EPA-rich polar lipid extract with 89.2% polar lipids and up to 39.6% EPA was obtained. This SL extract contained 80.1% of the GLs, 96% of the PLs and 67.8% of the EPA from the *Nannochlolopsis* sp. biomass. Good results were obtained combining the CO_2 SFE and PLE techniques as alternative green processes. Firstly, a lipidic fraction rich in NSLs (70.3% of the total extracted SLs) was obtained using supercritical CO_2 with 10 wt% ethanol as the co-solvent, at 35 MPa, 50ºC, 8 g CO_2/min for 8 h; this extract contained 81.7% of the biomass NSLs. Then, in the second extraction step with pressurized ethanol (96%), at 10 MPa, 125ºC and three extraction cycles of 5 min, an EPA-rich polar lipid extract with 85.1% polar lipids and up to 39.2% EPA was obtained. This SL extract contained 76.9% of the GLs, 71.1% of the PLs and 61.9% of the EPA from the *Nannochlolopsis* sp. biomass.

Keywords: microalga, polar lipid, eicosapentaenoic acid (EPA), supercritical fluid extraction (SFE), pressurized liquid extraction (PLE).

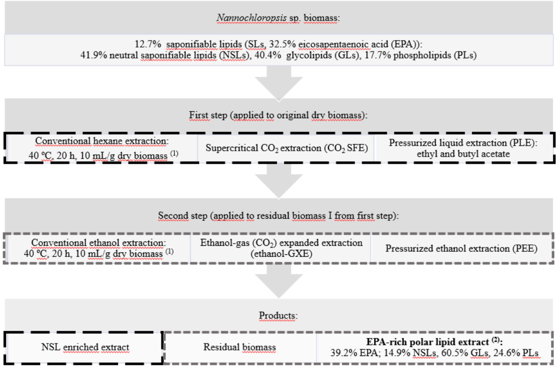

Figure 1: Scheme of the simultaneous extraction and fractionation of microalgal lipids from *Nannochloropsis* sp. lyophilized biomass in two steps by several extraction technicques. (1) Optimized conditions in previous work (Jiménez Callejón et al., 2020). (2) Best results attained in this work using green technologies.

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Time evolution of Molecular Binding in Mechanically controlled Break-Junctions

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[2] Instituto de Física de São Carlos, Universidade de São Paulo, Brazil
[3] Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany
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Abstract:

Mechanically controllable break junctions (MCBJs) are devices, in which the electrical properties of single molecules can be investigated with extreme precision using atomically structured metallic electrodes. The current-voltage (IV) characteristics in such junctions are considerably affected by the binding positions of the anchoring groups on the tip-facets and the configuration of the molecule. Hence, characterizing the electronic transport properties during a single tip-tip opening provides interesting insights in to the tip-molecule interaction.

In this contribution/poster, we present a novel, high-throughput approach to reproduce the time evolution of the electronic transport characteristics. For this, we performed transport calculations using the self-consistent charge scheme of the density-functional-based tight binding (SCC-DFTB)[1] approach and the Green's function formalism. In particular, we evaluated the energy level E_0 and the coupling Γ of the dominating transport channel using the single level model[2]. In contrast to standard approaches, we consider not just one molecule orientation but many thermodynamically relevant configurations. The obtained parameters were averaged using statistical weights obtained from Metropolis simulation considering up to 80.000 different configurations for selected tip-tip distances. The dependence of the averaged quantities with respect to the tip-tip separation reveals characteristic features also observed in experiments for similar molecular systems.

Our approach allows us to relate these features to binding-site and molecule-curvature effects and therefore provides a better interpretation of the experimental results.

Keywords: mechanically controlled break junctions, high-throughput simulations, density-functional-based tight binding, Salen, PEEB, single-level-model.

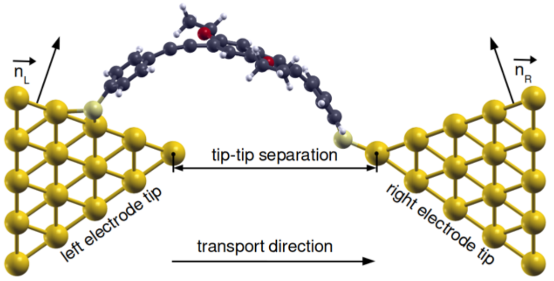

Figure 1: (a) Transport setup of a single PEEB molecule between gold electrodes. [PEEB = 1,4-bis(phenylethynyl)-2,5-bis(ethoxy)benzene]

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Process for the synthesis of nanostructures based on two-dimensional materials under concentrated solar irradiation

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Abstract:

The solar synthesis of nanostructures of 2D materials were performed through the solar irradiation of 2D-materials (C, TiO_2, MoS_2)[1,2] solid precursors under controlled atmosphere within the Heliotron reactor. The nanomaterials targeted have outstanding catalytic, thermal, lubricating, electronic and optical properties.

The process of such solar synthesis is non polluting, cost-effective and simple to implement. The inlet solar flux is reflected vertically in the axis of the parabola at the top which concentrates the incoming flux in a focal spot of 12mm. At this focal zone is placed in the pyrex balloon (for neutral atmosphere) the solid precursor set in various configurations (pellet, powder, pipe). The energy input is sufficient to heat-up the solid precursors until its melting and vaporization temperature.

Once vaporized the chemical species experience a slow temperature decrease allowing the nucleation process of nanoparticles before condensing themselves on the cold finger while the sweeping gas (Argon) is evacuated by the vacuum pump. The inner pressure and the solar power input have an impact on the size of synthesized powder and the yield of nanoparticles. The depositions on the cold finger form a powder easy to retrieve.

Keywords: 2D-materials, solar processes, nanomaterials synthesis.

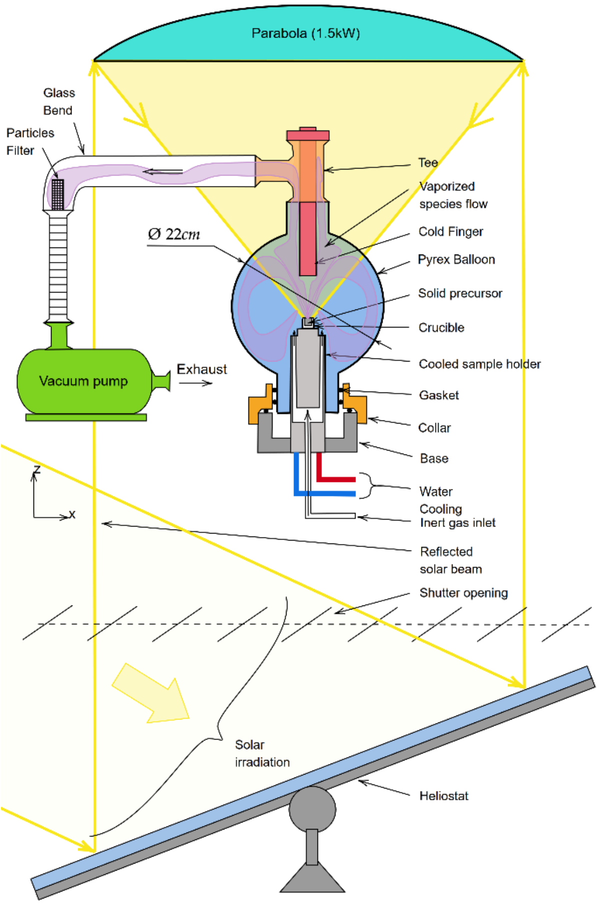

Figure 1: Detailed scheme of synthesis of nanomaterial within the Heliotron solar reactor.

References:

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Characterization of protein-utilizing group in anaerobic fermenters

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Abstract:

Anaerobic digestion (AD) is a promising technology to process protein-rich agro-industrial waste and wastewater. However, incomplete protein degradation during the acidification of organic matter is frequently observed when carbohydrates are present[1-3]. Little information on the mechanisms behind this phenomenon is provided in literature. This study further investigated the negative effect of carbohydrates on anaerobic protein degradation by restricting the carbon source fed to an anaerobic mixed culture. The obtained substrate conversion results were interpreted using microbial community analysis results. Two anaerobic fermenters fed with restrictive protein and/or carbohydrate substrates were operated and compared for the acidification and deamination processes, protease activity, and microbial community compositions. Results showed that when the restrictive carbon source was shifted from proteins to mixtures of proteins and carbohydrates, the degree of deamination in the protein-fed reactor decreased from 77% to 15% and the degree of acidification decreased from 75% to 34%. A decrease in protease activity was also observed. Anaerobic protein degradation was significantly retarded by the presence of carbohydrates. Microbial community analysis showed that microorganisms that can ferment both proteins and carbohydrates, i.e., generalists, were the predominant population in the microbial community (Figure 1), and they preferentially consumed carbohydrates. Therefore, the observed negative effect of carbohydrates on protein deamination and acidification could be mainly attributed by the preferential substrate utilization feature of these generalists. Further research on the metabolism functional analysis of the microbial community is recommended to confirm this finding. Overall, this study offers a better understanding of the mechanisms behind the negative effect of carbohydrates on protein degradation, which can provide insights into the design of the anaerobic digestion process of protein-rich wastewater.

Keywords: Anaerobic digestion, protein, carbohydrates, microbial community analysis.

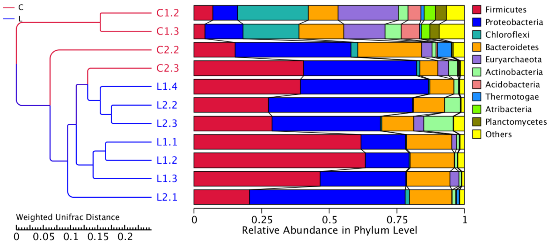

Figure 1: UPGMA cluster tree (left) and relative abundance of the top 10 phyla (right). C represents the protein-fed reactor, L represents the carbohydrates-fed reactor: C1.2, stage I (day 62); C1.3, stage I (day 84); C2.2 and C2.3, stage II (day 132); L1.1, stage I (day 8); L1.2, stage I (day 62); L1.3 and L1.4, stage I (day 84); L2.1, stage II (day 112); L2.2 and L2.3, stage II (day 132). In stage I, C-reactor was fed with casein and L-reactor was fed with lactose; in stage II, both reactors were fed with a mixture of proteins and carbohydrates. The top 10 phyla are displayed in the different color bar, the rest are grouped into the ''others'' and displayed in the yellow bar.

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