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### Speaker Abstracts

#### The Influence of Oxygen Physisorption on Two-dimensional Rhenium Diselenide Photodiodes

Nitzan Cohen, Yarden Mazal Jahn and Assaf Ya'akovovitz\*

*Ben-Gurion University of the Negev, Israel*

##### Abstract

Photodiodes are key components in opto-electronic systems. Two-dimensional (2D) rhenium diselenide (ReSe<sub>2</sub>) offers new prospects in such devices due to its thickness-independent, moderate, and direct p type bandgap. We show here that the physisorption of oxygen plays an instrumental role in chemical doping of the ReSe<sub>2</sub>, as it enhances the positive charge carrier conductivity. We characterized the electrical and opto-electrical responses of a few-layered ReSe<sub>2</sub> and ReSe<sub>2</sub>/hexagonal boron-nitride (h-BN) heterojunction under different conditions of gating and illumination. While the h-BN encapsulation did not change the excitonic nature and atomic bonds of the ReSe<sub>2</sub>, it prevented its oxygen physisorption, and as a result, considerably deteriorated its conductivity. On the other hand, ReSe<sub>2</sub> photo detectors that physisorbed ambient oxygen experienced enhancement of their conductivity and, therefore, showed improved performances with high currents, excellent responsivity, detectivity, and external quantum efficiency. Thus, this work sheds light on the fundamental physics of ReSe<sub>2</sub>. We manipulated the conductivity of ReSe<sub>2</sub> via its oxygen doping, thereby emphasizing the importance of ambient exposure to the successful operation of ReSe<sub>2</sub> as a high-end opto-electronic component.

#### X-ray Scattering Metrology for Analyzing Dispersivity and Crystallinity of Magnetite Nanoparticles

Valeria K.C. Molina, Tárisis M. Germano, Bruna P. Lima, Giancarlo E.S. Brito and S.L. Morelhão\*

*Institute of Physics, University of São Paulo, Brazil*

##### Abstract

Control of shape and size dispersivity and crystallinity of nanoparticles (NPs) has been a challenge in identifying these parameters' role in the physical and chemical properties of NPs. There are many examples, such as improved catalytic performance of cerium(IV) oxide NPs by adjusting size, morphology, and lattice perfection, tuned non-linear optical response in bismuth ferrite nanocrystals for biomedical imaging applications by narrowing phase and size dispersivity, and self-stabilized catalysts based on NPs with crystalline core and amorphous shell. The need for reliable quantitative tools for analyzing the dispersivity and crystallinity of NPs is a considerable problem in optimizing scalable synthesis routes capable of controlling NP properties. The most common tools are electron microscopy and X-ray scattering techniques. However, each technique has different susceptibility to these parameters, implying that more than one technique is necessary to characterize NP systems with minimum reliability. Wide-angle X-ray scattering (WAXS) is mandatory to access information on crystallinity. In contrast, electron microscopy (EM) or small-angle X-ray scattering (SAXS) is required to access information on the whole

NP sizes. EM provides average values on relatively small ensembles compared to bulk values accessed by X-ray techniques. Besides the fact of SAXS and WAXS weight size distribution differently, SAXS is easily affected by NP-NP interactions. Addressing the long-standing challenge of cross-analyzing data from techniques with different sensitivities to nanoparticle parameters, we now present an improved SAXS/WAXS-based methodology, building upon our previous work, to provide reliable quantitative results for dispersivity and crystallinity in magnetite NPs.

## Strain Engineering of the Mechanical Properties of Two-dimensional Tungsten disulfide

Yarden Mazal Jahn<sup>1</sup>, Guy Alboteanu<sup>1</sup>, Dan Mordechai<sup>2</sup> and Assaf Ya'akovovitz<sup>1</sup>

<sup>1</sup>Faculty of Engineering Sciences, Ben-Gurion University of the Negev, Israel

<sup>2</sup>Faculty of Mechanical Engineering, Technion – Israel Institute of Technology, Israel

### Abstract

Tuning the physical properties of two-dimensional (2D) materials is crucial for their successful integration into advanced applications. While strain engineering has demonstrated an efficient means to modulate the electrical and optical properties of 2D materials, tuning their mechanical properties has not been explored. In this work, we applied compressive strain through the buckling metrology to 2D tungsten disulfide (WS<sub>2</sub>). In this method, a controlled uniaxial strain is transferred from a compliant substrate to a thin film, and the deformed (wrinkled) shape of the latter is used to extract its elastic properties. We studied the behavior of few-layered WS<sub>2</sub> flakes under compressive strains ranging between 0.3% to 4%. We demonstrated mechanical softening manifested by the reduction of the effective Young's modulus of WS<sub>2</sub>. We performed in-situ Raman spectra experiments, in which we acquired the Raman spectra of strained WS<sub>2</sub> samples (compressive strain ranged from 0% to 2%). Due to compression, all peak positions (A<sub>1</sub>-, E<sub>2g</sub>'<sup>+</sup>) and E<sub>2g</sub>'<sup>-</sup> modes) redshifted with the increasing strain, indicating vibrational modes softening in the WS<sub>2</sub>. This observation agrees with the mechanical softening observed in our buckling experiment. In parallel, we conducted a molecular dynamics simulation that confirmed the validity of continuum mechanics modeling in the nanoscale and revealed that, due to sequential atomic-scale buckling events in compressed WS<sub>2</sub>, it exhibits mechanical softening. Therefore, by tuning the mechanical properties of WS<sub>2</sub> we shed light on its fundamental physics, thus making it an attractive material for high-end applications, from tunable sensors to flexible opto-electronic devices.

## Evaluation of the Physical Chemistry Interface Properties of the Bitumen by Contact Angles

Paolino Caputo<sup>1</sup>, Pietro Calandra<sup>2</sup>, Salvatore Procopio<sup>1</sup>, Ruggero Angelico<sup>3</sup>, Giorgio Celebre<sup>1</sup> and Cesare Oliviero Rossi<sup>1</sup>

<sup>1</sup>Department of Chemistry and Chemical Technologies, University of Calabria, Italy

<sup>2</sup>CNR-ISMN, National Research Council, Institute for the Study of Nanostructured Materials, Italy

<sup>3</sup>Department of Agricultural, Environmental and Food Sciences, University of Molise, Italy

### Abstract

This study aimed to investigate the warm mix mechanism of surfactant-based warm mix additives. The effects of the warm mix additive on the conventional physical properties, viscosity-temperature characteristics, and steady-state viscous flow properties of bitumen were investigated. Then, based on the theory of surface energy, the effects of the warm mix additive on the surface free energy of bitumen were investigated by contact angle measurements. Additionally, this technique was used to analyze the adhesion between bitumen and aggregate, and this interaction was systematically examined. The effect of the warm mix additive on the microstructure of bitumen was studied by atomic force microscopy and Young's modulus analysis.

## Graphene a Powerful Antioxidant Agent for Bitumen

Paolino Caputo<sup>1</sup>, Valeria Loise<sup>1</sup>, Pietro Calandra<sup>2</sup>, Salvatore Procopio<sup>1</sup>, Bagdat Teltayev<sup>3</sup> and Cesare Oliviero Rossi<sup>1\*</sup>

<sup>1</sup>Department of Chemistry and Chemical Technologies, University of Calabria, Italy

<sup>2</sup>CNR-ISMN, National Research Council, Institute for the Study of Nanostructured Materials, Italy

<sup>3</sup>Joldasbekov Institute of Mechanics and Engineering, Kazakhstan

### Abstract

In recent times, circular economic initiatives answering the need for sustainable materials have brought about several attempts at the eco-friendly, eco-sustainable and cost-effective production of asphalt pavements. It is an increasingly common practice in the asphalt industry to improve road pavement performance using additives to enhance the physio-chemical properties of bitumen, i.e., the binding material in the asphalt mix. This paper evaluated the potential of graphene additive as a modifier and antioxidant agent for bitumen. Samples of neat, aged and doped aged bitumen were analyzed. In this study, the amorphous carbon, graphene and graphite additives (commercial additives, Iterchimica company is acknowledged for providing materials) were characterized in terms of structure, which was correlated with the mechanical properties of the tested samples. The mechanical properties of the neat, modified, aged and unaged samples were evaluated via Dynamic Shear Rheology, atomic force microscopy, confocal and optical microscopy. Graphene proved to be excellent antiaging and can improve the properties of bitumen binder and the performance of asphalt pavements in general.

## Modeling Statistical Structural Disorder in Molecular Beam Epitaxy-grown Aluminum Gallium Arsenide/Gallium Arsenide Superlattices for Quantum Bragg Mirrors Using Synchrotron X-ray Diffraction

Mateus T. e Souza<sup>1</sup>, Germano M. Penello<sup>1</sup>, L.A.T. de Souza<sup>1</sup>, A. Alzeidan<sup>1</sup>, Andre A. Quivy<sup>1</sup>, M. Baksi<sup>2</sup>, P.J. Simmonds<sup>2</sup> and Sérgio L. Morelhao<sup>1\*</sup>

<sup>1</sup>Institute of Physics, University of São Paulo, Brazil

<sup>2</sup>Electrical and Computer Engineering, Tufts University, USA

### Abstract

Aluminum Gallium Arsenide/Gallium Arsenide (AlGaAs/GaAs) superlattices grown by molecular beam epitaxy (MBE) are foundational for advanced opto-electronic devices, including quantum Bragg mirror (QBM) based infrared detectors. The performance of such devices critically depends on achieving near-perfect periodicity and abrupt interfaces within the multilayer stack. However, intrinsic statistical fluctuations in layer thickness and composition during MBE growth introduce structural disorder, potentially degrading device efficiency and yield. Understanding and quantifying this nanoscale disorder is therefore essential for optimizing growth protocols and predicting device characteristics. This study presents a detailed analysis of structural disorder in a 20-period superlattice designed for QBM applications. High-resolution structural characterization was performed using high-energy (25 keV) synchrotron X-ray diffraction at the Sirius light source. Q-scans along the surface normal direction provided detailed information on the superlattice periodicity and layer structure. Advanced line profile analysis, employing a kinematic diffraction model refined via simulated annealing, was utilized to extract statistical parameters describing the layer fluctuations. The analysis revealed average layer thicknesses close to nominal values but quantified significant statistical deviations: standard deviations in GaAs and AlGaAs layer thicknesses were found to be  $\sigma_{\text{GaAs}} \approx 0.4$  nm and  $\sigma_{\text{AlGaAs}} \approx 0.5$  nm, respectively, with a standard deviation in Al composition  $\sigma_x \approx 0.02$ . Furthermore, evidence suggests these fluctuations exhibit a short-range correlation extending over approximately 2 - 3 superlattice periods. This quantitative characterization of nanoscale structural disorder provides crucial feedback for MBE process refinement and enables more accurate modeling of QBM device performance, linking fundamental growth phenomena to device-relevant properties.

## Cubic $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ Quantum Wells by Molecular Beam Epitaxy

Erik Antonio Arroyo Sosa\*, Marlene Camacho Reynoso, Yuriy Kudriavtsev, Máximo López López, Luis Martin Reséndiz Mendoza and Yenny Lucero Casallas Moreno

*Interdisciplinary Professional Unit in Engineering and Advanced Technologies, National Polytechnic Institute, Mexico*

### Abstract

The cubic-phase  $\text{In}_x\text{Ga}_{1-x}\text{N}$  alloy is a promising and viable alternative for solid-state lighting applications, particularly in light-emitting diodes (LEDs). The potential of this ternary material arises from its direct bandgap, which spans a broad range of the solar spectrum, from the InN bandgap (0.56 eV) to that of GaN (3.23 eV) at room temperature. This study reports the growth of cubic (metastable)  $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$  quantum wells (QWs) using molecular beam epitaxy on GaAs (001) substrates. Three QWs were deposited per sample, each with a thickness of 10 nm and GaN barriers of 30 nm. Secondary ion mass spectrometry was employed to assess chemical abruptness and determine the In (x) concentration in the QWs. Additionally, X-ray photoelectron spectroscopy provided insights into the binding energies within the cubic  $\text{In}_x\text{Ga}_{1-x}\text{N}$  QWs. Photoluminescence measurements revealed energy transitions within the visible spectrum, particularly in the green region, in agreement with theoretical calculations. These findings contribute to the development of high-performance active regions for LEDs.

## Isomerization of Tetra-(ortho)-substituted 4-aminoazobenzene in Cetyltrimethylammonium Bromide Micelles

Sandra Ramírez-Rave<sup>1\*</sup>, Natalia Rincón-Londoño<sup>2</sup>, Alberto S. Luviano<sup>3</sup> and Anatoly K. Yatsimirsky<sup>1</sup>

<sup>1</sup>*Faculty of Chemistry, National Autonomous University of Mexico, México*

<sup>2</sup>*Department of Engineering Physics, Division of Science and Engineering, University of Guanajuato, México*

<sup>3</sup>*Department of Chemical, Electronic and Biomedical Engineering, Division of Science and Engineering, University of Guanajuato, México*

### Abstract

Photo switchable molecules, such as azobenzene, have garnered significant attention due to their remarkable photo responsive ability to alter their conformation. These compounds are typically synthesized in their thermodynamically stable transformation, which can be converted into the metastable cis configuration upon exposure to light of an appropriate wavelength. The isomerization process can be finely tuned by rationally designing the substituent moieties within their molecular structure. A particularly intriguing aspect is the interaction of azobenzene with condensed matter systems like micelles. Understanding these interactions provides valuable insights into the behavior of azobenzene in confined environments. Furthermore, these photo switchable molecules exhibit the potential to modulate micellar systems under light stimuli, offering promising applications in responsive materials and controlled delivery systems. Here, we present a family of tetra-(ortho)-substituted 4-aminoazobenzene derivatives containing 2,6-dimethoxy groups in the 4-aminobenzene ring and either 2',6'-methoxymethyl (1), 2',6'-dimethyl (2), 2',6'-HH (3), or 2',6'-dichloro (4) groups in the second aromatic ring. These derivatives interact with cetyltrimethylammonium bromide micelles, adopting different conformations in spherical and wormlike micellar structures. We demonstrate that the isomerization reaction occurs either inside or outside the micelles, depending on the nature of the substituents in the azobenzene structure, significantly influencing the micellar physiochemical environment. Not only were rheological alterations observed, but physiochemical properties such as the pKa and rates of the isomerization reaction of the different azobenzene were also affected as a result of the interaction between these photo switches and the macromolecular environment of the tested micelles.

## Functional Nanomaterials in Life Sciences and Opto-electronics: Bottom-up Approaches for a Rational Design

Sara Cerra\*, Tommaso A. Salamone, Martina Mercurio, Beatrice Pennacchi and Ilaria Fratoddi

*Sapienza University of Rome, Italy*

### Abstract

Materials in the nanoscale range exhibit fascinating properties compared to their bulk counterparts, *i.e.*, light absorption and scattering, high surface-to-volume ratio, surface reactivity, electrical, and magnetic properties. Among these, functionalized noble metal nanoparticles (MNPs), metal oxide, polymeric nanoparticles and nanocomposites depict a suitable platform for developing multi-functional responsive systems with applications from opto-electronics to life sciences. Plasmonic nanoparticles, *i.e.*, gold, silver, and palladium nanoparticles (AuNPs, AgNPs, PdNPs), and metal oxide nanoparticles, *i.e.*, titanium dioxide and ferric oxide (TiO<sub>2</sub>NPs, Fe<sub>2</sub>O<sub>3</sub>NPs) bear several advantages: tunable size, ease of surface functionalization, and colloidal stability. Particularly attracting are their optical properties based on the localized surface plasmon resonance phenomenon and peculiar antibacterial properties. The synthetic versatility allows their functionalization with neutral or charged, hydrophilic or hydrophobic, organic or organometallic mono- and bi-functional thiols, both used single or in a mixture. Moreover, MNPs can be manipulated to induce self-assembly into complex structures, 2D or 3D networks that show collective properties. Besides, hydrophilic polymeric NPs synthesized by radical polymerization of vinyl monomers can be used as nanocarriers in the biomedical field. Conventional and advanced morpho structural studies were performed to study structure–function relationships to rationally design nanomaterials for future applications.

## Exploring the Role of Nickel and Iron in Shaping the Physical Properties of Multifunctional Porous Glass-based Nanocomposites

Agnieszka Cizman\*

*Wroclaw University of Science and Technology, Department of Experimental Physics, Wroclaw, Poland*

### Abstract

The ability to fabricate materials at the nanometer scale has opened new avenues for both industry and scientific research. The growing demand for materials with enhanced physical, chemical, and mechanical properties alongside precise dimensional control is one of the primary drivers behind material miniaturization. The development of nanomaterials for advanced technological applications requires mastery of both fabrication processes and a wide array of characterization techniques. Materials science has thus become a particularly dynamic field, spurred by the emergence of novel materials, cutting-edge manufacturing methods, and complex scientific challenges. In this presentation, a novel method for fabricating a new class of ferroic and multiferroic nanocomposites based on porous glass matrices will be discussed. These materials exhibit both ferroelectric and ferromagnetic properties and were synthesized by filling magnetic porous glasses with selected ferroic materials. Comprehensive investigations of the electrical, thermal, and magnetic properties were conducted on both the empty magnetic glass matrices and the resulting nanocomposites. The low electrical conductivity of the ferromagnetic porous glass enabled detailed dielectric, electromagnetic, and magnetoelectric measurements offering a major advantage for studying such systems. Magnetization measurements confirmed the ferromagnetic nature of several multiferroic nanocomposites, and for all composites studied, anomalies associated with the Verwey phase transition were observed. A particularly important result of this study was the discovery of a non-monotonic dependence of the ferroic phase transition temperature on pore size. This behavior is characteristic of ferroelectric systems in which surface layer polarization exceeds volume polarization. Notably, the presented results constitute the first experimental investigation of the size effect in ferroic crystals over such a wide range of particle sizes. Further structural analysis, including surface morphology and pore-filling factor evaluation, enabled determination of key physical parameters for both the porous glasses and the resulting nanocomposites. Moreover, the interaction between the glass matrix and the embedded ferroic phases and its influence on size-dependent effects was examined in detail. These findings provide valuable insights into the structure–property relationships of novel multiferroic composites and significantly advance the understanding of size effects in ferroic materials embedded in disordered porous matrices. To date,

a comprehensive theoretical model describing such systems is still lacking. The results presented here offer a new perspective on the mechanisms governing ferroic behavior at the nanoscale in complex composite systems.

## The Nanocomposite Design Strategies of Plant Wings

Benny Bar-On\*

*Department of Mechanical Engineering, Ben-Gurion University of the Negev, Israel*

### Abstract

Biomechanical plant parts are structured as hierarchical materials, fundamentally made of nanocomposite building blocks of helical cellulose nanofibrils and a hemicellulose matrix. The nanomechanical characteristics of these composite building blocks are functionally modified, locally adapted, and globally upscaled to provide the overall plant part with specialized load-bearing characteristics. In my talk, I will introduce the nanocomposite design of spinning seeds, explore their nanoscale elastic characterization by nanoindentation, and discuss the upscaling strategies of these nanoscale properties to form a mechanically supreme, ultra-thin wing element. These natural composite-material design principles may pave the way toward advanced synthetic forms of tunable aeronautical materials for various engineering applications.

## Quantification of Total Reactive Oxygen Species in Ultrafine Bubble Water Using the Dichloro-dihydro-fluorescein diacetate Fluorescence Assay

Thuy Linh Ha\*, Masatoshi Yoshimura and Itaru Sotome

*The University of Tokyo, Japan*

### Abstract

Ultrafine bubbles (UFBs) have emerged as promising agents for enhancing seed germination, although their effects may vary depending on species-specific oxidative stress responses. However, methods for directly quantifying reactive oxygen species (ROS) in UFB water remain limited. This study employed the 2',7'-dichlorodihydrofluorescein diacetate (DCFH-DA) fluorescence assay to evaluate total ROS levels in UFB water. DCFH (the deacetylated form) was prepared via alkaline hydrolysis of DCFH-DA, diluted with phosphate-buffered saline, and used at a final concentration of 10  $\mu$ M. Equal volumes of DCFH and water samples were mixed (1:1), including distilled water (DW), UFB1 ( $4.8 \times 10^7$  particles/ml), and UFB2 ( $1.09 \times 10^8$  particles/ml). Three water samples (DW, UFB1, and UFB2) and a DCFH-only control (no water added) were measured for fluorescence intensity at excitation/emission wavelengths of 502/523 nm. The DCFH-only control showed the highest fluorescence (6692 RFU), followed by UFB2 (5592 RFU), UFB1 (4953 RFU), and DW (4703 RFU). The increasing fluorescence trend (DW < UFB1 < UFB2) indicates a positive correlation between UFB concentration and ROS levels in water. These findings demonstrate the applicability of the DCFH-DA assay for detecting ROS in UFB water and provide a basis for future studies on seed responses to UFB-induced oxidative stress.

## Thermoelectric and Photovoltaic Properties of Copper-Copper(II) Oxide-Cuprous Oxide- Zinc Oxide Heterostructures for Energy Harvesting

Davis Gavars<sup>1,2\*</sup>, Margarita Volkova<sup>1</sup>, Raimonds Meija<sup>1</sup>, Artis Kons<sup>2</sup>, Donats Erts<sup>1</sup> and Jana Andzane<sup>1</sup>

<sup>1</sup>*Institute of Chemical Physics, University of Latvia, Latvia*

<sup>2</sup>*Faculty of Medicine and Life Sciences, University of Latvia, Latvia*

### Abstract

The ever-increasing necessity for greener energy production makes the conceptualization and production of new

energy-harvesting materials an important part of the transition from fossil fuels. Metal oxides, like copper(II) oxide (CuO), cuprous oxide (Cu<sub>2</sub>O), and zinc oxide (ZnO) exhibit thermoelectric, photovoltaic, and catalytic properties similar to those of other widely known materials (e.g., bismuth selenide (Bi<sub>2</sub>Se<sub>3</sub>), cadmium telluride (CdTe)), while being more readily available, more cost-effective, and less toxic. In this research, through the nano structuring of copper oxides and fabrication of a ZnO layer on top, a multifunctional heterostructured material, where a p-n junction can exist between the Cu<sub>2</sub>O and ZnO layers, was fabricated to utilize their thermoelectric and photovoltaic energy harvesting capabilities from solar light. The heterostructure was synthesized by first oxidizing copper foil in air to produce CuO nanowires, which were then partially reduced to Cu<sub>2</sub>O by annealing in a vacuum. A crystalline layer of zinc was then deposited on the partially reduced copper oxide nanowires via physical vapor deposition and subsequently oxidized in air to produce ZnO. A scanning electron microscope (SEM) equipped with an energy-dispersive X-ray analyzer was used to characterize the morphology and chemical composition of the material. X-ray diffraction analysis was performed to identify the crystalline composition of the material. The heterostructure's capability to generate voltage was tested both in a vacuum (in-situ SEM using a SmarAct 13D nanomanipulator) and under ambient conditions, through photovoltaic and thermoelectric measurements under illumination from specific wavelengths across the visible-infrared spectrum, including infrared, red, green and blue light-emitting diodes.

## Smart Nanostructured Materials as Drug Delivery Vehicles to Treat Cancer, Kidney and Cardiovascular Diseases

Hermis Iatrou<sup>1</sup>, Iro Kyroglou<sup>1</sup>, Iren Stavrakaki<sup>1</sup>, Cristina Varfi<sup>1</sup>, Pandora Thimi<sup>1</sup>, Dimitrios Skourtis<sup>1</sup>, Maria Kasimatis<sup>1</sup>, Konstantinos Dimas<sup>2</sup>, Dimitris Vlassopoulos<sup>3</sup> and Iordanis Mmourouzis<sup>4</sup>

<sup>1</sup>Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece

<sup>2</sup>Department of Pharmacology, Faculty of Medicine, University of Thessaly, Larissa, Greece

<sup>3</sup>Department of Materials Science & Technology, Institute for Electronic Structure and Laser, Greece

<sup>4</sup>Division of Pharmacology, National and Kapodistrian University of Athens, Athens, Greece

### Abstract

Novel, multifunctional nanoparticles (NPs) and hydrogels that exhibit a unique set of properties for the effective treatment of cancer are presented. The materials are comprised of polypeptide and polyethylene oxide (PEO) polymers that are non-cytotoxic polymers. The amphiphilic hybrid materials assemble in aqueous media to form micelles or vesicles, comprised of an outer hydrophilic corona of PEO chains, as well as a pH- and redox-responsive hydrophobic core. Dynamic light scattering, static light scattering, and transmission electron microscopy were utilized to obtain the structure of the NPs. Moreover, the pH- and redox-responsiveness in the presence of the reductive tripeptide of glutathione was investigated at the empty as well as the loaded NPs. The ability of the synthesized polymers to mimic natural proteins was examined by circular dichroism, while the study of zeta potential revealed the "stealth" properties of NPs. The anticancer drug doxorubicin (DOX) was efficiently encapsulated in the hydrophobic core of the nanostructures. Finally, in vitro cytotoxicity assay of the DOX-loaded NPs against three different breast cancer cell lines showed that the nanocarriers exhibited better activity as compared to the free drug, rendering these novel NPs very promising materials for drug delivery applications. Hybrid-polypeptide materials formed injectable in situ, forming quickly self-healing hydrogels, responsive to alteration of pH and increase of temperature. The connection between the alteration of the secondary structure of the polypeptides with the viscoelastic behavior was revealed using rheology and circular dichroism. Small-angle neutron scattering and scanning electron microscopy were employed to shed light on the structure of the polymers and how it affects their rheological properties. The results suggest that these biomaterials have the potential to be used in several bio-applications such as drug delivery.

## Ultrasound-directed Biorthogonal Delivery of mRNA-loaded Lipid Nanoparticles

Emilio Di Ianni<sup>1\*</sup>, Jueun Jeon<sup>2</sup>, Huiyu Hu<sup>2</sup>, Jeremy M. Quintana<sup>2</sup>, Chanseo Lee<sup>2</sup>, Edwina Abou Haidar<sup>1</sup>, Sedra Mohammadi<sup>2</sup>, Ayrton Zargani-Piccardi<sup>1</sup>, Mohammed Mahamdeh<sup>3</sup>, Iván Coto Hernández<sup>4</sup>, Thomas S.C. Ng<sup>2,5</sup>, Koen Breyne<sup>1</sup>, Hakho Lee<sup>2,4,5</sup>, Xandra O. Breakefield<sup>1</sup> and Miles A. Miller<sup>2,5</sup>

<sup>1</sup>Department of Neurology, Molecular Neurogenetics Unit, Massachusetts General Hospital, Harvard Medical School, USA

<sup>2</sup>Center for Systems Biology, Massachusetts General Hospital Research Institute, Boston, USA

<sup>3</sup>Cardiology Division, Cardiovascular Research Center, Massachusetts General Hospital, Harvard Medical School, USA

<sup>4</sup>Institute for Innovation in Imaging, Massachusetts General Hospital, Harvard Medical School, USA

<sup>5</sup>Department of Radiology, Massachusetts General Hospital, Harvard Medical School, USA

### Abstract

Delivery of mRNA with lipid nanoparticles (mRNA-LNPs) holds transformative potential for treating a range of diseases, but efficient, site-specific delivery to extrahepatic tissues remains a major challenge. Conventional targeting approaches, such as antibody conjugation, rely on high levels of surface receptors with favorable trafficking, which are often absent or heterogeneously expressed in target tissues. To overcome this limitation, we developed a flexible, receptor-independent targeting platform based on membrane-anchored bio-orthogonal chemistry. We developed amphiphilic click-reactive anchors (ACRAs) by conjugating the fusogenic lipid dioleoyl-phosphatidylethanolamine (DOPE) to either the click handles trans-cyclooctene (TCO) or its reactive counterpart, methyl-tetrazine (mTz), forming ACRA-TCO and ACRA-mTz. ACRA-TCO spontaneously incorporates into cell membranes, displaying TCO moieties on the surface and enabling subsequent reaction with mTz-bearing molecules. *In vitro*, ACRA-TCO achieved efficient and stable membrane labeling and rapid bio-orthogonal reactions with mTz-functionalized probes. To enable spatiotemporal control of membrane labeling, ACRA-TCO was encapsulated into ultrasound-responsive nanobubbles. Upon focused ultrasound (FUS) exposure, nanobubble cavitation released ACRA-TCO locally, anchoring clickable moieties to nearby cell membranes and generating a click-reactive membrane surface for selective mRNA-LNP capture. When administered systemically *in vivo*, ACRA-mTz-modified mRNA-LNPs bound efficiently to TCO-labeled cells, were internalized, and significantly enhanced local mRNA delivery and protein expression. This modular strategy integrates biomaterials engineering, click chemistry, and focused ultrasound to overcome the inherent limitations of receptor-based targeting. ACRAs enable precise, site-specific, and image-guided delivery of mRNA-LNPs to extrahepatic tissues, offering a clinically translatable platform for advancing gene therapies.

## Stabilization and Dynamics of Skyrmions in Stepped Nanowires for Multistate Memory Devices

W. Al Saidi<sup>1\*</sup> and R. Sbiaa<sup>2</sup>

<sup>1</sup>Unit of Physics, College of Applied Sciences and Pharmacy, University of Technology and Applied Sciences, Oman

<sup>2</sup>Department of Physics, College of Science, Sultan Qaboos University, Oman

### Abstract

Magnetic skyrmions are localized, non-uniform magnetization textures exhibiting topological stability and exceptional promise as information carriers in spintronic devices. Among their most prominent applications is racetrack memory (SkRM), where digital information is encoded via the presence or absence of a skyrmion. However, conventional ferromagnetic SkRM faces two critical limitations: (i) the non-uniform spacing between skyrmions, leading to bit misalignment, and (ii) the skyrmion hall effect, which causes lateral drift during motion. To address these challenges, this study investigates skyrmion dynamics in stepped (constricted) nanowires. The results demonstrate that geometric constrictions significantly influence skyrmion stability and mobility, inducing velocity reduction and helical trajectories within the constricted regions. These findings confirm that nanoscale engineering can effectively regulate skyrmion behavior. Furthermore, by extending the study to the case of two skyrmions, it is shown that repulsive interactions—both inter-skyrmion and edge-induced—restrict the system to one stable skyrmion per confinement region. This controlled behavior enables the development of multistate memory architecture. Notably, the system demonstrates the feasibility of achieving eight discrete memory states within seven confined regions using polarized current pulses. These insights pave the way toward robust, high-density, and energy-efficient skyrmion-based memory devices.

## Scenario Oriented Strategies for Phosphorus Management by Using Environmental Nanotechnology

Yanyang Zhang<sup>1,2\*</sup>, Chao Shan<sup>1,2</sup> and Bingcai Pan<sup>1,2</sup>

<sup>1</sup>State Key Laboratory of Pollution Control and Resource Reuse, School of Environment, Nanjing University, China

<sup>2</sup>Research Center for Environmental Nanotechnology, Nanjing University, China

### Abstract

Phosphorus (P) is the determinant factor of eutrophication and a critical element for human life. However, P is also a finite resource on earth that will deplete in 100 years. In order to close the P loop from human perspective, researchers have developed enormous technologies for P removal and recovery, among which the nano-enabled technologies are the most promising candidates. Despite the efforts, P pollution still persists worldwide, which calls for reflections on recent developments, as well as the coming challenges and opportunities in the near future. In this presentation, we intend to elaborate on our scenario-based environmental nanotechnology for P advanced treatment, P recovery, and P immobilization, highlighting the cutting-edge developments and discoveries that best fit the purpose of each scenario. A series of polymeric, carbon-based and clay-based nanocomposite materials developed by our team will be introduced. Their synthesis, structure, reactivity, P management capability and corresponding mechanisms at various scenarios (including wastewater treatment plants, rivers and lakes, industries, as well as the corresponding P recovery potential) will be discussed. This presentation also summarizes the merits and impacts of nanotechnology with a focus on nanoconfinement effects (e.g., size, stability, crystallization) and long-term structural evolution of nanocomposite materials during real-world applications. The influence of P species (e.g., phosphate, phosphonates, organophosphate esters), co-existing substances, solution chemistry and reactor configurations on the structure and reactivity of nanocomposite materials will be elaborated in detail. Finally, we envision the paths for future research and practical application.

## Assessment of Heavy Metal Adsorption: Comparative Analysis Between Silver Nanoparticles Fabricated from Coffee Oil and Frankincense Oil

Widad Al Rawahi\*, Amatur Roquia, Sahab Abdullah Al-Riyami, Zakiya Ahmed Al-Mawali, Ahed Issa Al-Hashmi and Wedad Hamed Al-Gheilani

University of Technology and Applied Sciences, Oman

### Abstract

Green synthesis of nanoparticles offers a sustainable and eco-friendly alternative to conventional chemical methods. The aim of this study is to compare the adsorption of lead by silver nanoparticles synthesized using different plants extracts (coffee oil and Al Hojari frankincense). Coffee oil and Al Hojari frankincense oil were extracted using Soxhlet extractor and hexane as a solvent. The yield of Al Hojari frankincense oil was significantly higher than the coffee oil. Nanoparticles were synthesized from coffee oil and Al Hojari frankincense, whereas the quantity of silver nanoparticles from coffee was doubled silver nanoparticles. Silver nanoparticles from Al-Hojary frankincense and coffee oil were synthesized and analyzed by fourier transform infrared spectroscopy and differences were found in which some of the peaks such as hydroxide ion are present in one and absent in the other. This is due to the presence of different compounds in the plant extract which might be left active during the extraction process and interact with the silver ions ( $\text{Ag}^+$ ) and incorporated on the surface of AgNPs. Scanning electron microscope and X-ray diffraction show the differences in the size of AgNPs particles and their crystallinity. The adsorption of lead using the synthesized nanoparticles was investigated where different factors that affect the adsorption were studied. The highest adsorption of lead by AgNPs synthesized using frankincense oil was found at the following conditions: pH 7, 15 °C and 30 min for the contact time compared to pH of 10.5, 50 °C and 45 min whereas the highest adsorption of lead by AgNPs synthesized using coffee oil.

## Extraction of Cellulose Nanocrystals from Textile Waste for Wastewater Treatment: A Circular Economy Approach

Asma Al Hosni\*, Widad Al Rawahi, Yumna Al-Shoukria and Ghadeer Al-Bahrانيا

*University of Technology and Applied Sciences, Sultanate of Oman*

### Abstract

The global textile industry is a major contributor to environmental degradation, driven by the rise of disposable fashion and the resulting surge in textile waste. This study presents a circular economic approach by extracting cellulose nanocrystals (CNCs) from cotton-based textile waste and evaluating their application in industrial wastewater treatment. Using acid hydrolysis, the process achieved a high yield of CNCs, contributing to both waste valorization and environmental sustainability. The extracted CNCs were characterized using fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and scanning electron microscope (SEM), confirming their structural integrity and suitability for environmental applications. FTIR analysis revealed functional groups essential for heavy metal interactions, while XRD patterns indicated a well-defined crystalline structure with an increased crystalline index, enhancing stability and adsorption capacity. SEM images showcased the nanoscale dimensions and surface characteristics conducive to effective adsorption processes. The CNCs exhibited excellent adsorption capabilities for lead, primarily through physical interactions driven by electrostatic forces. This project highlights a viable method for waste management and underscores the potential of CNCs as eco-friendly adsorbents for industrial wastewater treatment, contributing to global sustainability goals. Future research could focus on optimizing extraction conditions and exploring surface modifications to enhance adsorption properties, further establishing CNCs as a promising solution for addressing heavy metal contamination in water.

## Seasonal Variations in the Toxicity of Urban Ultrafine Particles

C. Sioutas\*, Y. Aghaei, M. Badami, M. Aldakheel and R. Tohidi

*Department of Civil and Environmental Engineering, University of Southern California, California, USA*

### Abstract

The study was conducted to ascertain the toxicological characteristics and origins of ultrafine particles (UFPs) within the urban confines of Los Angeles. Employing a Dekati low-pressure impactor (DLPI), particles were collected across various size fractions, focusing notably on the ultrafine scale. This method was further enhanced by the integration of the DLPI with a versatile aerosol concentration enrichment system, which is known for its efficacy in concentrating ambient aerosols. Such an approach facilitated the precise assessment of the health impacts linked to different UFP size fractions. In assessing the oxidative potential of size-segregated UFPs, the dithiothreitol (DTT) assay was utilized alongside comprehensive chemical analyses, such as elemental carbon/organic carbon, metals, and inorganic ions. A rigorous source apportionment study was also undertaken to pinpoint the principal sources influencing the diverse UFP size ranges. Additionally, the research was expanded to include the use of a Sioutas Personal Cascade Impactor Sampler to gather particles in the accumulation mode range (0.25 - 2.5  $\mu\text{m}$ ), providing a comparative analysis of these particles' toxicity. Campaigns conducted during the winter and summer seasons were incorporated to explore the temporal variations in particle toxicity. The considerable variations observed in toxicity across different particle sizes offered essential insights into the differential toxicity of particulate matter. Consequently, the findings from this research not only advanced the understanding of the toxicological effects of airborne UFPs but also laid the groundwork for targeted interventions designed to alleviate the adverse health impacts of air pollution.

## Co-coagulation of Micro-Nano Bubbles for Enhanced Drinking Water Treatment: A Study on the Efficiency and Mechanism of a Novel Cleaning Process

Xiaojiang Huang<sup>1</sup>, Yao Huang<sup>1</sup>, Chengtao Yang<sup>1</sup> and Jinsuo Lu<sup>1,2</sup>

<sup>1</sup>School of Environmental and Municipal Engineering, Xi'an University of Architecture and Technology, China

<sup>2</sup>Shaanxi Key Laboratory of Environmental Engineering, Xi'an University of Architecture and Technology, China

### Abstract

Micro-nano bubbles (MNBs) are widely used in cleaning processes for environmental treatments, but few studies have examined the interaction of MNBs with coagulation. In this study, a novel process, i.e., MNBs-coagulation, was developed for enhanced drinking water treatment. The humic acid (HA) removal efficiency was used to evaluate the effectiveness of MNBs-coagulation for drinking water treatment. The hydrolysis component ratio of polymeric aluminum chloride (PACl) with and without MNBs, the complexation strength of HA and PACl, and flocculent functional group characterization were used to analyze the mechanism of the MNBs-coagulation process to enhance drinking water treatment. The results of a Jar test showed that the MNBs-coagulation process could improve the removal efficiency of HA (up to a 27.9% increase in dissolved organic carbon removal). In continuous-flow experiments to remove HA, MNBs-coagulation can increase the removal efficiency of UV254 by about 26.5% and with no significant change in turbidity. These results are attributed to the inherent hydroxyl radical generating properties of MNBs, the forced hydrolysis of PACl by MNBs to increase the Alcohol percentage, and the ability of MNBs to increase the complexation strength of HA with PACl. At the same time, the MNBs-coagulation process has a strong anti-interference ability, almost no interference from anions and cations such as Cl<sup>-</sup>, SO<sub>4</sub><sup>2-</sup> and Ca<sup>2+</sup>, and has a good performance in natural surface water. In summary, MNBs-coagulation has strong potential for practical applications to enhance the efficiency of drinking water treatment.

## Unraveling the Complex Stacking of Topological Insulator Mn<sub>x</sub>Bi<sub>2</sub>Te<sub>3+x</sub> Thin Films via Advanced Synchrotron X-ray Scattering

Maurício B. Estradiote<sup>1</sup>, Philipp Kagerer<sup>2</sup>, Celso I. Fornari<sup>2</sup>, Hendrik Bentmann<sup>2</sup>, Friedrich Reinert<sup>2</sup> and Sérgio L. Morelhao<sup>1\*</sup>

<sup>1</sup>Institute of Physics, University of São Paulo, Brazil

<sup>2</sup>Universität Würzburg, German

### Abstract

The precise control of structure and composition in topological insulator thin films like Mn<sub>x</sub>Bi<sub>2</sub>Te<sub>3+x</sub> (MBT) is paramount for their application in spintronics and other quantum devices. We introduce a generalized model to describe the structure of epitaxial MBT films on barium fluoride (111) substrates. This model, based on stacking probabilities of manganese bismuth telluride and bismuth telluride blocks, offers a complete framework for understanding film architecture across varying compositions, from pure phases to superlattice formation and phase segregation. We leverage the power of X-ray scattering, employing reciprocal space Q-scan simulations to identify structural fingerprints. These simulations reveal critical features sensitive to film structure, enabling quantitative analysis of composition and stacking order. High-flux synchrotron x-ray data, acquired at Deutsches Elektronen-Synchrotron, Petra III, beamline P08, confirmed our theoretical predictions, providing detailed structural and compositional insights. Beyond 1D Q-scans, 3D reciprocal space reconstruction methodologies were applied to uncover the lateral ordering within MBT films. Notably, this robust approach was also instrumental in investigating the synthesis of thulium telluride thin films on strontium fluoride (111) substrates another material system exhibiting topological states and strong electron correlations with significant potential for novel electronic and magnetic device development.

## Advanced Hybrid Nano-sources of Light for Nanophotonics

Renaud Bachelot<sup>1,2\*</sup>, Minyu Chen<sup>1</sup>, Yuqing Zhao<sup>1</sup>, Sylvie Marguet<sup>3</sup>, Ali Issa<sup>1</sup> and Safi Jradi<sup>1</sup>

<sup>1</sup>University of Technology of Troyes, France

<sup>2</sup>Nanyang Technological University, Singapore

<sup>3</sup>University of Paris Saclay, France

### Abstract

Rapid growth of the nanophotonic area requires the development of advanced nano sources of light whose geometry must be scalable with nanophotonic devices and whose tunability must be simple and efficient. Over the past two decades, hybrid plasmonic nano sources based on energy transfer between metal nanoparticles and quantum nano emitters have turned out to constitute a promising solution of efficient optical nano sources. We studied and exploited the nanoscale spatial positioning of semiconductor quantum emitters in the close vicinity of metal nanostructures. The control relies on plasmon-assisted nano-polymerization of a photosensitive formulation that hosts nano-emitters. Through selected examples, we show that this approach has opened promising new avenues, such as polarization-sensitive photoluminescence, lifetime engineering, control of the local space symmetry group, single photon switch that is driven by polarization, multicolor nano sources and chiral nano-emitters.

## Quasi-heterointerfaces and Electronic Structure in Sputtered Molybdenum Disulfide Films

Emilia S.W. Russell, Thomas C. Parker, Eva L.C. Benford, Eugene Pavlov, Dagou A. Zeze, Andrew J. Gallant and Iddo Amit\*

Department of Engineering, Durham University, Durham, United Kingdom

### Abstract

Scaling up the production of high-quality, large-area films of semiconducting transition metal dichalcogenides remains a significant challenge for their integration into mass manufacturing of electronic devices. Vapour phase manufacturing from elemental or oxide sources introduces complexity in both stoichiometric and chemical processing aspects, resulting in polycrystalline films with a high density of defects and random morphology. We utilize magnetron sputtering from a compound target for the direct deposition of large-area, high-quality films of molybdenum disulfide (MoS<sub>2</sub>) on various substrates, including silicon/silicon dioxide wafers and borosilicate glass. Our results demonstrate that sputtering from a compound target produces highly conductive films using power as low as 50W, followed by a thermally efficient annealing step. The second part of the presentation focuses on the electronic structure and internal interfaces of the sputtered MoS<sub>2</sub> films. Using a combination of macroscopic impedance measurements and Kelvin probe force microscopy, we show that thickness variations, resulting from local changes in layer count, can be attributed to the formation of abrupt quasi-heterointerfaces where free carrier and localized space charge densities govern charge transport mechanisms. Our experimental observations are contrasted with a stochastic lumped element model of nanoscale transport in polycrystalline materials. Here, random doping fluctuations induce local asymmetry in charge transport over the barriers. When expanded into large films, the model converges to a realistic probability density-based description of electronic behaviour, which will underpin future applications of these films.

## Molybdenum/Silicon Multilayers with Boron Carbide Interlayers and Titanium Dioxide Capping Layer for Extreme Ultraviolet Mirror

Chien-Cheng Kuo\*, Duy Thanh Cu, Kuan-Wei Lu, Kuan-Chieh Huang, Kuan-Yu Ko and Ai-Ling Shih

Department of Optics and Photonics, Thin Film Technology Center, National Central University, Taiwan

### Abstract

The yield of extreme ultraviolet (EUV) lithography technology is related to the EUV mirror. The thickness of the

interface diffusion layer and the surface roughness of the molybdenum/silicon multilayer mirror have a significant impact on the optical performance of the EUV mirror. This work was done by fine-tuning the ion beam parameters to achieve extremely low surface roughness, interface diffusion and well-controlled crystallization. The addition of an ultrathin boron carbide ( $B_4C$ ) barrier layer in the  $B_4C/Mo/B_4C/Si$  system significantly improves interface sharpness and suppresses asymmetric diffusion. Capping layer is applied to the EUV mirror using atomic layer deposition technology, and hydrogen ions generated by ion source to bombard the sample surface. Observing the capping layer can effectively prevent hydrogen ions from generating bubbles on the mirror surface and reducing the reflectivity. Using the titanium dioxide capping layer, the surface only showed slight undulations after 90 s of hydrogen ion bombardment, and the surface roughness was from 0.090 nm to 0.773 nm, indicating that it had a good inhibitory effect. Paving the way for the development of high-performance multilayer optical components for next-generation EUV lithography applications.

## Acceleration of Filler Network Development in Carbon-nanotube-filled Pastes to Enhance Electrical Conductivity for Printed Electronics Applications

Masahiro Inoue\* and Tomoya Hanada

Graduate School of Science and Engineering, Gunma University, Japan

### Abstract

Electrically conductive pastes containing carbon nanotubes (CNTs) are promising to be used for fabricating advanced microsystems by printed electronics technologies. Development of their electrical conductivity, called dynamic percolation, occurs during curing and post-annealing. The kinetics of dynamic percolation are controlled by variations in two factors, including the dispersion state of fillers and the interfacial electrical resistance between fillers. Thermosetting epoxy-based multi-wall CNT (MWCNT)-filled pastes exhibited dynamic percolation behavior governed by the development of interfacial conducting contacts to reduce electrical resistance between the fillers. A viscoelastic characterization for the curing process of the MWCNT-filled pastes showed a slight increase in storage modulus during gelation before the crosslinking of the binder molecules occurred, suggesting filler network formation through the interphase development. The interfacial electrical contact and the filler network formation were closely related to the dynamic percolation kinetics of the MWCNT-filled conductive pastes. The binder chemistry of the pastes can control these phenomena during curing and post-annealing; adding some mono-epoxy molecules effectively accelerates the kinetics of these phenomena. This paper discusses the effect of the molecular design for the additives on enhancing the dynamic percolation of the MWCNT-filled conductive pastes to establish material designs of advanced conductive pastes for applying printed electronics technologies.

## Drug Nanoforms: Cryochemical Production, Approach to Directed Drug Delivery and Controlled Drug Release

Tatyana I. Shabatina<sup>1,2\*</sup>, Yu.N. Morosov<sup>1,2</sup>, Irina V. Astashova<sup>3</sup> and Alexei V. Filinovskii<sup>2,3</sup>

<sup>1</sup>Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

<sup>2</sup>Faculty of Fundamental Sciences, Bauman Moscow Technical State University, Moscow, Russia

<sup>3</sup>Department of Mechanic and Mathematics, Lomonosov Moscow State University, Moscow, Russia

### Abstract

The use of medicinal substances in nanosized forms (nanoforms, nanoparticles) allows pharmaceutical preparations to increase their therapeutic effectiveness due to several factors: high specific surface area of nanomaterials, high concentration of surface-active centers interacting with biological objects. Cryochemical production is a powerful method of reducing the size of drug substances particles, changing their form and crystal structure in order to transfer them into nanoforms and improve their pharmaceutical properties. An application of this method allowed us to obtain antibiotics nanocrystals and their hybrid nanocomposites with metal particles. Antibacterial compositions were produced by low temperature drug and metal vapors co-deposition or cryogenic freeze-drying technique of mixed water solutions containing silver or copper nanoparticles and antibacterial components dioxidine or gentamicin. The thorough investigations transmission electron microscopy, electron diffraction, fourier transform infrared

spectroscopy, UV spectroscopy, X-ray diffraction, differential thermal analysis was made, it was shown that the hybrid compositions included silver and/or copper nanoparticles of 5 - 70 nm in diameter and nanoparticles of antibiotics of 50 - 250 nm in diameter. Cryochemical forms of drugs possess modified crystal structures and lower melting temperatures. New cryoformed hybrid composites of nanosized metal and antibiotic particles demonstrate higher antibacterial activity against *Escherichia coli* 52, *Staphylococcus aureus* 144, *Monomorium cyaneum* 98, *Bacillus cereus* 9 compared to the original drug substance and individual metal nanoparticles. The comprehensive mathematic models describing the different stages of cryomodification processes developed will give us the base for finding of the optimal values of different parameters for producing of drug nanoforms with desired therapeutic effects and bioavailability.

## Nanotechnology in Reproductive Biomedicine: Emerging Potentials and Cryoprotective Benefits of Nano-particles in Sperm Preservation

Burcu Esin\*

Universtiy of Ondokuz Mayıs, Turkey

### Abstract

Nanotechnology has gained increasing interest in reproductive biomedicine in recent years, offering promising applications in various areas such as gamete preservation, embryo development techniques, and fertility enhancement. Nanoparticle formulations, in particular, offer significant advantages in protecting sensitive cells such as spermatozoa due to their targeted effects at the cellular level, their ability to cope with oxidative stress, and their high bioavailability. Furthermore, nanoparticles are reportedly gaining widespread use in cryopreservation protocols due to their high antioxidant properties. Antioxidant defense system plays a crucial role in protecting sperm cells against lipid peroxidation and DNA damage. However, while traditional forms exhibit limited efficacy during intracellular uptake, nanoparticle forms can increase bioavailability and reduce toxicity. In this context, nanotechnological forms are considered a more effective and safer alternative to classical antioxidant strategies. There is extensive evidence in the literature that various nanoparticle antioxidant additives applied during semen cryopreservation contribute to preserving the functional and structural integrity of spermatozoa after freezing and thawing. These additives are reported to have positive effects on parameters critical to fertility, such as sperm motility, membrane integrity, morphology, and DNA integrity. Furthermore, it has been suggested that they may be effective in preserving the biological potential of sperm by reducing cellular damage caused by oxidative stress. These results demonstrate that the use of nanotechnology-assisted antioxidant forms can provide effective protection beyond traditional methods in sperm cryopreservation, suggesting that nanoparticle-based applications in reproductive biotechnology could be evaluated more broadly in the future.

## One-pot Microwave-assisted Synthesis of Carbon Dots and *In vivo* and *In vitro* Antimicrobial Photodynamic Applications

María Paulina Romero<sup>1\*</sup>, Fernanda Alves<sup>2</sup>, Mirian Denise Stringasci<sup>2</sup>, Hilde Harb Buzzá<sup>2</sup>, Heloísa Ciol<sup>2</sup>, Natalia Mayumi Inada<sup>2</sup> and Vanderlei Salvador Bagnato<sup>2,3</sup>

<sup>1</sup>Department of Materials, Faculty of Mechanical Engineering, National Polytechnic School, Ecuador

<sup>2</sup>São Carlos Institute of Physics, University of São Paulo, Brazil

<sup>3</sup>Hagler Fellow, Texas A and M University, College Station, United States

### Abstract

Carbon-based photosensitizers are more attractive than the other ones based on their low cost, high stability, broadband of light absorption, tunable emission spectra, high quantum yield, water solubility, high resistance to metabolic degradation, and selective delivery. These properties allow multiple applications in the field of biology and medicine. The present study evaluated *in vitro* and *in vivo* the antimicrobial photodynamic effect of a one-pot microwave produced C-DOTS based on citric acid. The *in vitro* assays assessed the effectiveness of illuminated C-DOTS (C-DOTS + light) against *Staphylococcus aureus* suspension and biofilm. The concentrations of 6.9 and 13.8 mg/mL of C-DOTS and light doses of 20 and 40 J/cm<sup>2</sup> were able to reduce significantly the microorganisms. Based on these parameters and results, the *in vivo* experiments were conducted in mice, evaluating this treatment on

wounds contaminated with *S. aureus*. The viability test showed that C-DOTS-mediated photodynamic inactivation reduced 10<sup>4</sup> logs of the bacteria present on the skin lesions. These results, altogether, showed that antibacterial photodynamic therapy using C-DOTS is a promising and viable treatment for Gram-positive bacteria infected wounds.

## **Outbreak Simulation on the Neonatal Ward Using Silica Nanoparticles with Encapsulated DNA: Unmasking of Key Spread Areas**

**M. Wallner<sup>1</sup>, Lara Pfuderer<sup>2</sup>, Lenka Bašková<sup>1</sup>, Kerstin Dollischel<sup>1</sup>, Robert Grass<sup>2</sup>, Andreas Kücher<sup>1</sup>, Anne Marie Luescher<sup>2</sup> and J.M. Kern<sup>1</sup>**

<sup>1</sup>*Institute of Clinical Microbiology and Hygiene, University Hospital Salzburg, Paracelsus Medical University, Salzburg, Austria*

<sup>2</sup>*Department of Chemistry and Applied Biosciences, Institute of Chemical Bioengineering, ETH Zurich, Zurich, Switzerland*

### **Abstract**

Nosocomial infections remain a major threat, especially in Neonatal Intensive Care Units (NICUs), where outbreaks often occur without sources or dynamics being fully understood. This study pioneers infection prevention research by using non-infectious nanoparticles (SPED: amorphous silica with encapsulated DNA) to simulate outbreaks in a real NICU environment. SPED can be tracked by polymerase chain reaction, enabling analysis of potential pathogen spread under real-life conditions. We showed that three distinct SPED DNAs, applied at three strategic points, could be detected for up to four days at multiple sampling sites. The observed dissemination patterns revealed the complexity of everyday spread in the NICU. Notably, the staff area emerged as a central hub: SPED introduced here rapidly dispersed to both staff areas and numerous patient rooms. In contrast, SPED applied within a single patient room spread only to staff zones, without reaching other patients' rooms. These findings identify the staff area as a critical node in outbreak dynamics—potentially misperceived as a “safe space” by staff and hygiene teams, but in fact a driver of transmission. Simulation studies with SPED thus offer a powerful tool to uncover hidden dynamics of microbial spread in hospitals. In the future, this approach may support the identification of outbreak trigger points and enable targeted hygiene measures, ultimately reducing nosocomial infections.

## **Optimizing the Average Distance Between a Blue Light Photosensitizer and a Harmonic Nanoparticle for Effective Infrared Photodynamic Therapy**

**Refael Minnes<sup>\*</sup> and Ayan Barbora**

*Faculty of Natural Sciences, Department of Physics, Ariel University, Ariel, Israel*

### **Abstract**

Photodynamic therapy can be significantly improved by techniques utilizing light windows of higher tissue penetration depths with optimally matched photoactive agents to provide deep interstitial treatment. Classical blue light photosensitizers were photodynamically activated using infrared light via coupled harmonic nanoparticles with optimized intermediary distances using spacers. Upon 800 nm pulsed laser irradiation perovskite nanoparticles with optimized coupling to either curcumin or protoporphyrin IX reduced the viability of MCF-7 breast cancer cells by 73% and 64% respectively, while exhibiting negligible dark toxicity. The findings pave the way for clinical adaptation of ease-of-synthesis photodynamically active preparations operable under deep tissue penetrating infrared lights using commonly available otherwise infrared inactive classical blue light photosensitizers.

## Deposition and Characterization of Silicon Dioxide Thin Films for Patterned Buried Graphene Nanofabrication

Sean Johnson\*, Tyler Rogers, Morgan Abrams, Sara Hamidpour and Vladimir Lagutin

High Point University, USA

### Abstract

Graphene, characterized by its unique thermal and electrical properties, is a two-dimensional carbon material with vast potential for flexible substrates, three-dimensional electronics, and enhanced photonics sensors with integration of nanowire (NW) photodetector applications. Selective area growth of NW on graphene is yet to be accomplished. In this study, thin film deposition methods were surveyed for effectiveness of thickness, precision, surface uniformity, and adhesion to graphene substrates for the purpose of burying graphene in a silicon dioxide (SiO<sub>2</sub>) dielectric layer. Radio-frequency sputtering resulted in a successful burial of graphene under a ~21 nm SiO<sub>2</sub> thin film. Raman spectroscopy was used to assess graphene's characteristics post-lithography and etching. The thickness measurements of the SiO<sub>2</sub> thin film were confirmed via ellipsometry and atomic force microscopy (AFM). Photolithography and reactive ion etching were used to fabricate the first patterns on buried graphene substrates. AFM results suggest successful exposure of the graphene, with potential application for controlled NW fabrication on graphene for photodetection using Si-based complementary metal-oxide-semiconductors technologies.

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