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TOPICS

- Photonics and Optoelectronics
- From Atoms to Devices: growth and fabrication
- Micro/Nano Electronics
- Low Dimensional Materials
- Magnetism and Strongly Correlated Systems
- Materials for Energy
- Soft Condensed Matter
- Advanced Functional Materials

PLENARY SPEAKER

- Prof. Emmanuel P. Giannelis, Cornell University

KEYNOTE SPEAKERS

- Prof. Natalie Stingelin, Georgia Tech.
- Prof. Wolfgang Heiss, Friedrich-Alexander-Universität
- Prof. Spiros H. Anastasiadis, University of Crete

INVITED SPEAKERS

- Prof. Maria Fyta, RWTH Aachen University
- Assoc. Prof. Pavlos S. Stephanou, Cyprus University of Technology
- Dr Spyros Kassavetis, Aristotle University of Thessaloniki
- Dr Marios Zacharias, Univ Rennes, INSA Rennes, CNRS
- Asst. Prof. Joan Papavasiliou, University of Patras
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SUNDAY 14 SEPTEMBER 2025

PLENARY TALK

Topic preference Advanced Functional Materials
Presentation preference (oral/poster): Plenary Talk
Full name of presenting author: Emmanuel P. Giannelis
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Development of Electrocatalysts for Energy Conversion and Storage Devices

Emmanuel P. Giannelis

Materials Science and Engineering, Cornell University

Abstract: Metal (including single atom) catalysts, SACs are critical components in a wide range of clean energy technologies, including water electrolysis and CO2 electro-reduction systems. In this talk, I will review our efforts to synthesize ultra-high surface area carbons by combining hypergolic reactions and a templated substrate with KOH activation. In addition, I will present the development of a family of SACs (Fe, Co, Cu) supported on nitrogen-rich hierarchical porous carbons using a) the templated pyrolysis of diaminopyridine, and b) a topotactic reaction using MOFs as precursors. Lastly, I will present and discuss the performance of these systems in a number of energy storage and conversion applications and compare to the state-of-the-art systems.

MONDAY 15 SEPTEMBER 2025

TALKS – SESSION 1

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Keynote Talk
Full name of presenting author: Spiros H. Anastasiadis
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Development of Superhydrophobic Polymer Nanocomposite Coatings with Antimicrobial Properties

Spiros H. Anastasiadis[1,2]

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Abstract: The development of antifouling and antimicrobial surfaces that would prevent the transfer of bacteria has gained the scientific interest during the recent years. In this work, polymer nanocomposite coatings are developed to provide surfaces with antifouling and antimicrobial properties. This was achieved via deposition of nanohybrid coatings containing the appropriate polymer and either alumina or titania nanoparticles or layered Mxene nano-additives or appropriate combinations of those. The coatings were deposited via dipping or spraying from aqueous dispersions on different substrates like stainless steel, glass and polypropylene to evaluate their wide utilization. The wetting properties were evaluated via contact angle and contact angle hysteresis measurements, the morphology of the coated surfaces was examined using Scanning Electron Microscopy (SEM), while the surface chemical composition was determined via Energy Dispersive Spectroscopy (EDS). The nanohybrid composition was optimized in order to achieve the desired wetting properties. For the optimized nanocoating compositions, a superhydrophobic (CA > 150°) and water repellent (hysteresis < 5°) surface was obtained. The stability of the coated surfaces with time or upon temperature treatment was examined whereas their antimicrobial properties were evaluated as well. Superhydrophobic and water repellent coatings using non-fluorinated polymers is achieved.

Acknowledgements: This research has been partially financed by the EU Horizon Europe Programme (project STOP [Grant Agreement 101057961] and project WISE [Grant Agreement 101138718]).

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Development of Dual-Mode SERS and Fluorescence Nanoprobes Using Mesoporous Silica-Coated Anisotropic Gold Nanoparticles

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Chrysafis Andreou[1]

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Abstract: Surface-enhanced Raman scattering (SERS) is a highly sensitive technique used for the detection of molecular species, relying on the amplification of Raman signals by localized surface plasmon resonance (LSPR) in metallic nanostructures. One of the most effective strategies in this field involves the design of SERS tags, which combine plasmonic nanoparticles with Raman reporter molecules to achieve strong, specific, and reproducible signals. Anisotropic nanoparticles, such as gold nanostars and nanoplates, are particularly efficient due to their sharp features and multiple plasmonic modes that generate intense electromagnetic hot spots.

Despite their advantages, these systems often suffer from limited stability and reduced analyte accessibility. Coating the nanostructures with a mesoporous silica shell addresses these issues by improving colloidal and chemical stability while preserving plasmonic properties. The porous architecture allows small analytes to diffuse through the silica layer and interact with the metallic core. Additionally, the silica surface provides a platform for functionalization with optical or bioactive molecules.

In this study, a coumarin-based fluorescent dye modified with a triethoxysilyl group is used to enable covalent incorporation into the silica matrix during the coating process. This approach ensures uniform dye distribution, prevents leaching, and allows the integration of fluorescence with SERS activity in a single nanosystem. The resulting hybrid probes offer dual-mode optical signals, enhancing detection reliability and versatility.

We present the synthesis and preliminary characterization of gold nanostars coated with mesoporous silica and functionalized with the silane-coumarin dye, as a proof of concept for the development of multifunctional platforms for SERS and fluorescence-based sensing.

Acknowledgments: This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No. 101034403

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
Full name of presenting author: Tamer M. Tamer
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Polystyrene and Sulfonated Derivatives for Ammonia Adsorption from Water

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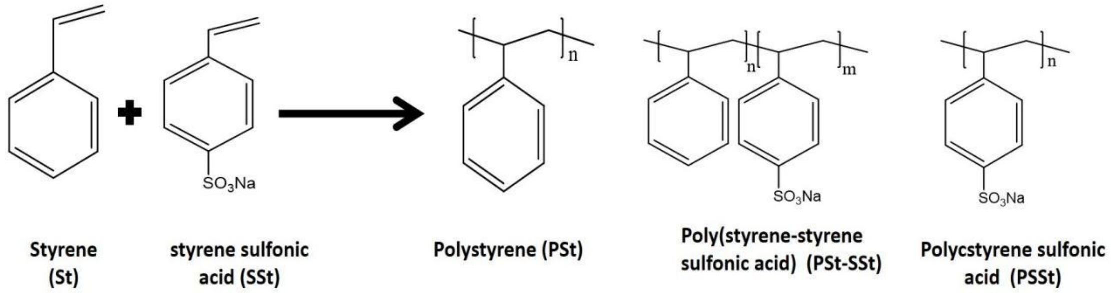
Abstract: The ab initio The removal of ammonia from aqueous environments is critical for environmental protection and the management of water quality. This study presents the synthesis and evaluation of a series of polymeric nanoparticles composed of polystyrene (PSt) and sulfonated polystyrene (PSSt) in various ratios (100:0, 90:10, 70:30, 50:50, and 0:100) for their ammonia adsorption performance. The nanoparticles were synthesized using a surfactant-free polymerization precipitation method and were thoroughly characterized through Fourier-transform infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), scanning electron microscopy (SEM), elemental analysis, ion exchange capacity (IEC), surface area analysis, and zeta potential measurements. The adsorption behavior of ammonia onto the nanoparticles was examined under varying operational conditions, including contact time, initial concentration, and temperature, to identify optimal parameters for removal efficiency. Furthermore, adsorption kinetics and thermodynamic parameters were analyzed to elucidate the underlying adsorption mechanisms and energy changes involved. The findings indicate the potential of sulfonated polystyrene-based nanoparticles as effective adsorbents for ammonia removal from water, thereby providing a promising approach for advanced water purification technologies.



Schematic preparation of polystyrene-styrene sulfonic acid copolymers

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Tuning the Performance of Sulfonated Polyvinylidene Fluoride-hexafluoropropylene/cellulose acetate Membrane by Sulfonic Acid Functionalized ZIF-8 for DMFC applications

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Abstract: A series of polymer-metal–organic framework (MOF) hybrid composite membranes were developed by integrating sulfonic acid-functionalized ZIF-8 (SO_3H-ZIF-8) with a matrix composed of sulfonated polyvinylidene fluoride-hexafluoropropylene (SPVDF-HFP) and cellulose acetate (CA). Sulfonation of PVDF-co-HFP was conducted by treating the copolymer with chlorosulfonic acid. The MOF was incorporated into the polymer matrix using a solution blending method, resulting in membranes with varying MOF concentrations. Detailed characterization of both the hybrid membranes and the pristine membranes was performed. Fourier-transform infrared spectroscopy and thermal analysis verified the chemical composition and thermal stability, while scanning electron microscopy confirmed uniform dispersion of MOF particles throughout the polymer matrix. Atomic force microscopy analyses revealed well-defined phase separation within the membrane structure. The inclusion of SO_3H-functionalized ZIF-8 significantly improved properties such as proton conductivity, water uptake, mechanical robustness, and dimensional stability without adversely affecting oxidative stability. Furthermore, single-cell evaluations demonstrated that the SO_3H-ZIF-8 composite membranes achieved higher proton conductivity and greater peak power density compared to the unmodified copolymer membranes.

Acknowledgment: We acknowledge the financial support of this work by the EU through the Recovery and Resilience Plan of the Slovak Republic within the framework of project no. “09I03-03-V04-00237”.

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Synthesis and Characterization of Polymer-Derived Carbon Foam for Solar Steam Generation

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Abstract: Carbon foams are candidate materials for energy and environmental applications. In this study, polymer-derived carbon foams were prepared through the controlled pyrolysis of melamine foams to deliver carbon foams that can be used as solar absorbers. It is found, that, optimized carbon foams can be prepared from a simple pyrolysis treatment and temperatures up to 1,000ºC. The efficiency of pyrolyzed products for solar heat absorption and evaporation of water is measured. In general, the carbon foams produced were characterized through scanning electron microscopy (SEM), elemental analysis (EDS), X-ray diffraction (XRD), and optical spectrometry (UV-Vis). Together with superior light absorptance (100%), ultrafast solar-thermal response (a temperature increase of 96.3°C within 2 mins under 0.7 sun), low thermal conductivity, and outstanding mechanical robustness, a high evaporation rate efficiency (2.6 Kg/W^{2}h at 1 sun) is achieved. The findings provide a new perspective in designing a functional material that satisfies the demand for eco-friendly, low-cost, highly efficient, and enduring solar steam generation.

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
Full name of presenting author: António Manuel de Bastos Pereira
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Mechanical Properties of Biaxial Non-Crimp Fabrics for 2-Wheeled Electrical Vehicle Chassis

António B. Pereira[1], Gabriel Constantinescu[1], Dina Silva[1], Ricardo Beja[1],
Mário Sousa Henriques[2]

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Abstract: The transition towards electric mobility has significantly increased the demand for sustainable materials that offer both strong mechanical performance and a reduced environmental footprint. In electric vehicle design, lightweight composite materials play a crucial role by decreasing overall vehicle mass, thereby improving both driving range and energy efficiency. Among these, natural fiber composites—such as those reinforced with flax or hemp—are gaining traction due to their renewability and lower environmental impact compared to conventional synthetic fibers like carbon and glass.
This study investigates the mechanical behavior—specifically tensile, compressive, shear, and flexural properties—of environmentally friendly biaxial non-crimp fabric composites for application in the chassis of two-wheeled electric vehicles. The materials examined include three fiber types: carbon, linen, and glass, each paired with a suitable resin matrix to produce structural laminates.
Mechanical testing was conducted in accordance with ISO standards, focusing on key parameters such as tensile strength, elastic modulus, Poisson's ratio, and strain. The carbon fiber composite, combined with a synthetic epoxy resin, demonstrated the highest performance, achieving a tensile strength of 1126 MPa. Linen-based composites, while offering a lower tensile strength of 351 MPa, showed the greatest strain at rupture, indicating superior ductility. Glass fiber composites recorded the lowest tensile strength at 102 MPa but provided moderate elasticity and ductility.
This research was conducted as part of the development of a next-generation smart electric scooter. The project emphasizes innovative structural design using low-impact or recycled materials, aiming to deliver both sustainability and aesthetic appeal. The mechanical data obtained will inform the numerical simulations used to optimize the scooter's frame design.

Acknowledgements: This work was developed in the scope of the Project AM2R – Agenda Mobilizadora para a inovação empresarial do setor das Duas Rodas" [C644866475-00000012 – project n. 15], financed by PRR – Recovery and Resilience Plan under the Next Generation EU from the European Union, and has laboratory support of the Centre for Mechanical Technology and Automation (TEMA).

MONDAY 15 SEPTEMBER 2025

TALKS – SESSION 2

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Keynote Talk
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Green flexible electronics — challenges and opportunities: A materials scientist's point of view

Natalie Stingelin

Georgia Institute of Technology, USA

Abstract: In recent years, immense efforts in the flexible electronics field have led to unprecedented progress in device engineering and the advancement of systems of ever-increasing performance. Despite these achievements, new materials design strategies are needed in order to widen the applications of flexible electronics technologies, expand their functionalities and features, with an increasing view on delivering sustainable solutions. We present here opportunities the use of multicomponent systems for, e.g., increasing the mechanical flexibility and stability of organic electronic products, introducing other features such as self-encapsulation and faster mixed ion-electron transport, and the beneficial effect on sustainability. One specific approach is based on blending polymeric insulators with organic semiconductors; which has led to a desired improvement of the mechanical properties of organic devices, producing in certain scenarios robust and stable architectures. We also discuss the working principle of semiconductor:insulator blends, examining the different approaches that have recently been reported in literature. We illustrate how organic field-effect transistors (OFET)s and organic solar cells (OPV)s can be fabricated with such systems without detrimental effects on the resulting device characteristics even at high contents of the insulator, while detrimental effects on the environment can be decreased. Furthermore, we review how blending can assist in the fabrication of more reliable and versatile organic electrochemical transistors (OECT)s.

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Progress in the fabrication of sustainable thin-film solar cells using pulsed laser deposition

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Abstract: Solar power is now an established source of clean and renewable energy production, contributing to the global efforts to reverse climate change. Among the variety of solar-photovoltaic technologies, thin-film solar cells have recently become the focus of intensive development, due to their unique combination of advantages. Chief among them are CIGS-based solar cells, that exhibit high conversion efficiency (23.35%), high radiation resistance, and outstanding stability. They are also thin, light, and can be manufactured on flexible substrates.

However, state-of-the-art CIGS-based solar cells have two drawbacks. Firstly, they require a variety of techniques for the deposition of their constituent layers. Secondly, they contain rare and toxic materials. In the pursuit of a solution to both these disadvantages, this work reports on the utilization of pulsed laser deposition (PLD) as a single technique for the preparation of the active layers of a complete solar cell, using only abundant and safe materials.

Employing a single deposition technique greatly reduces manufacturing complexity. At the same time, exploiting the recent scaling and commercialization of PLD, it potentially decreases processing time and fabrication costs through streamlined production lines. Recently, CZTS cells have been manufactured with over 10% efficiency. Hence, replacing the CIGS absorber with CZTS and testing alternative materials for the other layers, enables the substitution of the toxic (Mo, Cd) and rare (In, Ga) elements in the stack.

The results presented herein discuss the methodology followed toward the realization of this objective and the progress achieved. The structural, compositional, morphological, electrical, and optical characteristics of the PLD-grown thin films were parametrically investigated through pertinent techniques, such as X-ray diffraction, energy-dispersive X-ray spectroscopy, Hall effect measurements, photoluminescence, etc. This investigation enabled the correlation of PLD process parameters to film properties, thus leading to optimization of the constituent layers for the fabrication of a complete solar cell.

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
Full name of presenting author: Christina Lekka
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Biocompatible β-Ti-based alloys for bone implants

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[2]Department of Chemistry, University of Torino, Torino, Italy
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Abstract: Beta-type Ti-based alloys has been promising for bone implants due to their low Young moduli, high corrosion resistance and minimal cytotoxicity while their enrichment with well-known antibacterial elements like Ga, Cu and Ag causes antibiofilm activity. This work presents Density Functional Theory calculations using Siesta or Vasp software on Ti-based alloys aiming to reveal the electronic origin of the structural and mechanical properties, for the design of materials with predefined properties, even antibacterial, suitable for hard tissue implant applications. Ab-initio results reveal the suitable electronic properties while the calculated mechanical stability conditions and the elastic constants predict the a'-TiNb stabilization only for Nb-rich compositions and the known w-shape Young modulus curve in agreement with the experimental data. The enrichment of beta-TiNb with selective elements like In and Sn might decrease the Young modulus while Ga and Ag provide antibacterial characteristics. Furthermore, metallic implants require surface treatment which would be friendly for the adsorption and growth of human mesenchymal stem cells (hMSCs) promoting therefore the bone formation. To this end the simulation of adhesion and migration of hMSCs on β-Ti -based surfaces using large scale simulations with the Hybrid Cellular Potts model aims to mimic the experimental data. The diffusion coefficient and the hMSC- surface pattered sizes are directly correlated while the elongation and lamellipodium behaviour is simulated in line with experimental data. These results could be used for the design of a micropatterned biocompatible and antibacterial surface suitable for hMSCs adsorption, proliferation, and osteogenic differentiation for orthopedic and dental implants.

Acknowledgements: This work is supported by the Bioremia project (H2020-MSCA-ITN-2019, No 861046, 2020-2024).

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Synthesis and Characterization of Bimetallic Oxides

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Abstract: This presentation focuses on the synthesis of rare-earth zirconate nanomaterials with the general $Ln_2Zr_2O_7$, where Ln(III) = La, Nd, Dy, and Gd, and the bimetallic $NiFe_2O_4$ nanomaterials. These bimetallic oxides were synthesized in the form of nanopowders, xerogels, and aerogels, enabling a comparative study of their structural characteristics and properties. A comprehensive analysis was conducted using techniques such as X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), N_2 adsorption−desorption porosimetry, differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA). By compiling all structural data, we showed that, in addition to the chemical composition, the synthetic method and drying protocol have a major impact on the final structural characteristics of the nanostructured materials. Powders were synthesized via co-precipitation, while wet gels were prepared via the sol−gel technique. Ambient drying of wet gels led to xerogels and drying in supercritical CO_2 led to aerogels. Our findings suggest that the synthesized powders consist of nanoparticles arranged in a dense microstructure with a very small specific surface area and porosity. In contrast, xerogels and the aerogels are composed of nanometer-sized globular structures. The xerogels exhibit microporosity, whereas the aerogels demonstrate a wide pore size distribution, highlighting the influence of the drying process on their porous architecture.

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Sustainable Adhesive Systems Based on Reinforced Aleppo Pine Resin: A Thermal and Mechanical Study

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Abstract The increasing demand for bio-based materials in industrial applications has driven interest in the development of natural adhesives with enhanced performance. This study explores the potential of Aleppo pine resin (Pinus halepensis, PH) and its composites, modified with nano- and micro-scale additives, as sustainable adhesive systems for wood bonding. Three types of fillers were incorporated into the raw resin: carbon black (CB) nanoparticles, organo-modified montmorillonite clay (CL), and biomass-derived ash (BA). Their effect on the resin's thermal stability and mechanical strength was evaluated using thermogravimetric analysis (TGA), scanning electron microscopy (SEM), and lap shear tests performed on wooden substrates according to ASTM D1002. The lap shear results demonstrated that resin modifications significantly enhanced bonding strength, with PH/CB and PH/CL composites yielding the greatest increases–up to 22.2% and 16.5% over the unmodified resin (Table 1).

Table 1: Results of lap shear tests

Sample	Mean Smax (Mpa)	SD	Percentage (%) increase
PH	1,090	0,040	-
PH/CB 1%	1,264	0,065	16,0
PH/CB 2%	1,332	0,046	22,2
PH/CL 1%	1,221	0,054	12,0
PH/CL 2%	1,270	0,054	16,5
PH/BA 1%	1,112	0,056	2,1
PH/BA 2%	1,169	0,032	7,3

Thermal analysis (Table 2) revealed a consistent three-phase degradation profile among all samples. Minor mass loss (0-12%) was recorded below 120 °C, attributed to volatiles. Between 120 °C and 260 °C, differences emerged depending on the filler, with BA-containing samples showing the highest intermediate weight loss. Major decomposition occurred in the 260–450 °C range, with total losses exceeding 85% across all groups. Notably, the onset decomposition temperature ($T_{5\%}$) declined in most composite systems, indicating a trade-off between early thermal activation and improved bonding. Peak degradation temperatures (T_{max}) spanned 308–322 °C, while residual mass at 600 °C varied between 3.5% and 9.5%, reflecting the influence of inorganic fillers.

Table 2: Results of thermal stability measurements

Weight - loss stages	PH	PH/CB 1%	PH/CB 2%	PH/CL 1%	PH/CL 2%	PH/BA 1%	PH/BA 2%
First *(below 120 °C)*	0%	0%	5%	0%	7%	12%	2%
Second *(120 - 260 °C)*	10%	10%	14%	12%	21%	26%	16%
Third *(260 - 450 °C)*	93%	85%	91%	85%	94%	85%	93%
$T_{5\%}$ *(°C)*	221	229	120	206	109	98	145
T_{max} *(°C)*	316	316	320	322	315	308	318
Residual weight % *(600 °C)*	3,5	7,2	6,7	9,5	3,7	6,7	3,7

The findings support the use of modified Aleppo pine resin as a viable alternative to synthetic adhesives for wood and composite applications.

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Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Scattering properties of water wave metamaterials: from submerged structures to shallow water theory

C. Marangos

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Abstract: Water wave metamaterials, composed of closely spaced periodic vertical barriers, are engineered to manipulate wave propagation through structured microgeometry. These systems share conceptual parallels with their electromagnetic and acoustic counterparts, where sub-wavelength microstructures induce effective medium behavior such as negative refraction and cloaking. Their analysis relies on homogenisation and multi-scale expansions to capture the large-scale effects of the small-scale structure.

In our work, we derive a model for a three-dimensional submerged water wave metamaterial using homogenisation, asymptotic analysis, and perturbation techniques. The structure consists of vertical barriers protruding from the seabed but remaining fully submerged. The resulting effective medium captures complex scattering behavior, such as negative refraction and total internal reflection. This model extends previous two-dimensional configurations where the barriers reach the free surface and shows strong agreement with those models, while diverging from predictions based on shallow water theory.

When the same metamaterial microstructure is placed within a shallow water regime, a new derivation is required due to the interplay of multiple small parameters: shallowness, narrowness, and wave amplitude. Starting from first principles, we develop a novel multi-scale asymptotic framework to derive a simplified yet accurate two-dimensional model. This analytically solvable system reveals how the scattering properties—such as negative refraction and reflectionless waveguiding through curved channels—are directly linked to the design parameters. The model provides a powerful and explicit tool for the design and analysis of wave manipulation in shallow water environments using metamaterial-inspired structures.

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MONDAY 15 SEPTEMBER 2025

TALKS – SESSION 3

Topic preference: Materials for Energy
Presentation preference (oral/poster): Invited Talk
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Energy storage in supercapacitors based on biomass residues

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Abstract: The increasing energy demands in portable applications are driving research towards the development of advanced energy storage devices, reliable and environmentally friendly. In recent years, supercapacitors based on carbon electrodes with a large specific surface area (electrochemical double layer capacitors, EDLCs) have been developed for applications that require high energy in short periods of time, as they exhibit high power density, good performance and long lifetime, compared to batteries. Their use in hybrid and electric vehicles, in electronic systems, in aircraft and also in smart networks has spread. Supercapacitors could work great in conjunction with batteries and fuel cells in hybrid systems to improve regenerative braking or the ability to produce more acceleration through their ability to discharge quickly. Considering some of the advantages such as low cost, large specific surface area and high conductivity, activated carbons are considered as the ideal material for the preparation of electrodes for supercapacitors. Especially in the case where the activated carbon comes from biomass, the benefits of the circular economy are added to the advantages of this particular arrangement. The biochars resulting from the use of residual biomass can, depending on their preparation technique, have an interconnected network of mesopores, providing efficient pathways for the transport of ions and their diffusion. In the last decade, the technological directions in the field of biomass, both at European and national level, have focused on the energy utilization mainly of plant residues (e.g. sawdust, fruit peels, nut shells, olive kernel etc.) with the development of new and improved energy conversion technologies with high degrees of efficiency, thus facilitating the transition from the linear to the circular economy. The world's biomass potential, being to a large extent intact, could fully cover the planet's energy demands.

Topic preference: Materials for Energy
Presentation preference (oral/poster): Oral
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Thermoelectric PEDOT:PSS films with $Bi_{0.4}Sb_{1.6}Te_3$ made via drop-casting

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Keywords: low temperature thermoelectrics, PEDOT:PSS, conductive polymer, thermoelectric films

Abstract: Organic-based thermoelectric materials have gained interest in alternative low-temperature thermoelectric applications instead of the classic inorganic materials due to their intrinsic advantages as polymers. Some of these advantages of conductive polymers are the low thermal conductivity, abundance, easy processability, low-toxicity and cost-effectiveness. The main advantages that support the use of thermoelectric polymer-based materials in such applications are their tuneable electrical properties via various additives and processing methods along with their inherent flexibility that broadens the thermoelectric applications field with more novel device designs and application varieties. An example of such polymers is PEDOT:PSS due to its high electrical conductivity, compared to other polymers, that is tuneable with various simple doping methods that can modulate its morphology by separating PEDOT and PSS polymers to improve carrier mobility. Additionally, it has a comparatively higher Seebeck coefficient, due to the bipolaron network with asymmetric density of states at Fermi level, and a low thermal conductivity originating from weak lattice vibrations.

This work studies the thermoelectric performance of PEDOT:PSS based films deposited on glass substrates via drop-casting and the effect of additives such as organic solvent DMSO, inorganic thermoelectric $Bi_{0.4}Sb_{1.6}Te_3$ along with HCl. These show the effects of modulating the morphology and also the effect of incorporating inorganic additives in conductive polymer films on its thermoelectric performance. The study is done by means of Seebeck coefficient and electrical conductivity measurements to calculate the material power factor across a temperature range, showing significant improvements depending on the additive and its concentration.

Topic preference: Materials for Energy
Presentation preference (oral/poster): Oral
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Self-Healing Solid Polymer Electrolytes Based on Nanostructured Polymer Particles for Solid-Sate Batteries

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Abstract: As the demand for high-performance and sustainable energy storage solutions intensifies, solid-state battery (SSB) technologies are gaining critical importance. Among recent innovations, self-healing polymer electrolytes-capable of autonomously repairing physical damage—offer significant advantages by extending battery lifespan and enhancing operational safety. Here, we present a novel class of self-healing solid polymer electrolytes composed of hard–soft multiphase nanostructured polymer particles as additives to a fast ion-conducting polymer matrix. These nanostructured particles form a percolated network that reinforces mechanical integrity while incorporating fast dynamic healing motifs that enable rapid autonomous repair. This macromolecular design effectively addresses two central challenges in SPE development: (i) the inherent trade-off between ionic conductivity and mechanical strength, and (ii) the conflict between mechanical robustness and healing efficiency in conventional self-healing systems. Our approach offers a versatile platform for designing next-generation solid polymer electrolytes that are simultaneously strong, conductive, and rapidly self-healable—key attributes for the advancement of safe and durable solid-state batteries.

Acknowledgements: The research work was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the “RRF: Basic Research Financing (Horizontal support for all Sciences), Sub-action 1. Funding New Researchers –” (Project Number: 15955).

Ελλάδα 2.0 ΕΘΝΙΚΟ ΣΧΕΔΙΟ ΑΝΑΚΑΜΨΗΣ ΚΑΙ ΑΝΘΕΚΤΙΚΟΤΗΤΑΣ
Με τη χρηματοδότηση της Ευρωπαϊκής Ένωσης NextGenerationEU
ΕΛ.Ι.Δ.Ε.Κ. Ελληνικό Ίδρυμα Έρευνας & Καινοτομίας

Topic preference: Materials for Energy
Presentation preference (oral/poster): Oral
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Structure-Property Relationship of Biocompatible and Biodegradable Diblock Copolymer Electrolytes Based on Polyhistidine and Polyethylene Oxide

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Abstract: The increasing need for sustainable alternatives to petrochemical-based polymers has driven significant interest in bio-based polymers. These materials offer promising solutions to environmental concerns while enabling applications across various fields, from everyday consumer products to high-performance technologies. In this study, we investigate polypeptides with different architectures—homopolymers and block copolymers with polyethylene oxide—as polymer electrolytes for lithium battery applications. A comprehensive structure–property relationship analysis is conducted, focusing on ionic conductivity, thermal properties, and mechanical strength in polypeptide-lithium salt systems. Small-angle (SAXS) and wide-angle (WAXS) X-ray scattering techniques are employed to elucidate the material’s structural organization, while ionic conductivity is assessed via electrochemical impedance spectroscopy. Thermal behavior is examined using differential scanning calorimetry (DSC), and rheological studies provide insights into mechanical performance. The findings of this work contribute to the development of bio-based polymer electrolytes with tailored properties for next-generation energy storage applications.

Acknowledgements: The research work was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the “RRF: Basic Research Financing (Horizontal support for all Sciences), Sub-action 1. Funding New Researchers –” (Project Number: 15955).

TUESDAY 16 SEPTEMBER 2025

TALKS – SESSION 1

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Keynote Talk
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Defect tolerance in halide perovskites

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Abstract: In the view of photovoltaic-devices it almost a magic that the best halide perovskite solar cells, which are based on polycrystalline thin films, to date reach almost the same power conversion efficiency as the best silicon heterostructure solar cells, based on high quality single crystalline wafers. In literature there are several special properties of the lead halide perovskites are discussed to be the reason for the astonishing good performance of the especially lead halide perovskites in respect to their optoelectronic properties. The first idea of these has been “defect tolerance” claiming that defect tolerance is the tendency of a semiconductor to keep its properties despite the presence of crystallographic defects. While this idea was initially supported by theoretical predictions about defect energies and their emission and capturing cross sections, meanwhile “defect tolerance” is under question to be present in halide-perovskites, at least from a theoretical stand point of view. Thus, verifications are needed, which are based on experiments that provide both, defect densities as well as capture cross sections. Reviewing such experimental attempts, suggests also that a much clearer definition of what defect tolerance indeed could mean, is required [1]. Such a definition has to include for instance the type of defect the perovskites can tolerate, the density range of defects under question, and a standard material to compare the tolerant behavior. Independent of defect tolerance or not, defect passivation strategies are successful in lead-halide perovksites, for which examples will be presented in this talk, based on epitaxially grown microcrystalline perovskite laser devices, as well as on roll-to-roll printed perovskite solar cells.

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Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Invited Talk
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Tailoring solid state nanopores via computational modelling

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Abstract: Solid state nanopores are nanometer-sized openings in materials of different types and thicknesses. These can electrophoretically drive charged (bio)molecules by means of an applied voltage difference. The transport of the analytes is strongly dependent on the interplay of the electrophoretic and the electroosmotic forces generated within the nanopores and gives rise to measurable ionic and/or electronic currents along and across the pores. Using computer simulations at diverse spatiotemporal scales, we model the transport of different analytes, such as single and molecular ions, DNA molecules and short peptides though solid state nanopores. For the latter, we probe 2D materials, such as graphene and molybdenum disulfide, as well as novel Janus type materials. The simulations allow us to obtain a detailed atomistic insight into the exact interactions of the nanopore material, the analyte, and the surrounding liquid environment. We discuss these insights in the concept of DNA sequencing, detection of post-translational modifications in proteins, desalination and blue energy generation.

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Acknowledgements

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Topic preference: Materials for Energy
Presentation preference (oral/poster): Oral
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Enhancing the Performance of Flexible Printed Perovskite Solar Cells via Modified PEDOT:PSS Hole Transport Layers

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Abstract: In recent years, Perovskite Solar Cells (PSCs) have emerged as a key point in photovoltaic technology due to their outstanding power conversion efficiency and extensive light absorption range. Their ability for low-cost, scalable fabrication on lightweight and flexible substrates -especially through printing techniques- further advances their potential to become the mainstream high-efficiency PV technology. In inverted PSC architectures, a good alignment between the Highest Occupied Molecular Orbital (HOMO) energy level of the hole transport layer (HTL) and that of the perovskite layer is essential for efficient hole transport. However, the energy mismatch between PEDOT:PSS and $MAPbI_3$ often leads to energy losses, ultimately limiting device performance. In this work, a modified PEDOT:PSS (m-PEDOT:PSS) formulation was developed and its integration in PSCs as the HTL was investigated, in order to understand the effect on the PSC device performance. A polymer electrolyte was added in different concentrations in a commercially available PEDOT:PSS solution and the resulting m-PEDOT:PSS HTLs were slot-die coated on flexible IMI/PET substrates. All modified PEDOT:PSS nanolayers showed low roughness, higher transmittance and better energy level alignment with the perovskite, compared to PEDOT:PSS nanolayers. Finally, fully printed flexible PSC devices using m-PEDOT:PSS as the HTL were fabricated using slot-die coating and these devices exhibited significantly higher PCE and improved overall performance compared to devices using a PEDOT:PSS HTL.

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Topic preference: Materials for Energy
Presentation preference (oral/poster): Oral
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Impact of Doped Fullerene Buffer Layers On The Performance of Perovskite Photovoltaics

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Abstract: Inverted PSCs incorporate solution processed $PC_{70}BM$ as the ETL, which offers good electron charge extraction and passivation of the perovskite active layer grain boundaries. Thick fullerene diffusion-blocking layers could benefit the lifetime of inverted PSCs. In a previous work we have shown that by increasing the thickness of $PC_{70}BM$ the thermal stability of inverted PSCs is improved under accelerated thermal conditions [Galatopoulos *et al*. Long Thermal Stability of Inverted Perovskite Photovoltaics Incorporating Fullerene-Based Diffusion Blocking Layer. *Adv. Mater. Interfaces* 5, (2018)]. However, the low conductivity of $PC_{70}BM$ leads to a drop of the PV parameters, thus limiting the applicability of thick (200 nm) $PC_{70}BM$ buffer layer for optimized PSCs performance. In this presentation, we show that by applying N-DMBI doping we can maintain the PCE of PSCs with thick $PC_{70}BM$ diffusion blocking layer. Importantly, 0.3 % w.t. N-DMBI doped 200 nm $PC_{70}BM$ diffusion blocking layer based inverted PCSs retain a high thermal stability at 60 ^{O}C of up to 1000 h without sacrificing their PCE photovoltaic parameters. [Galatopoulos, F *et al*. Optimized Doping of Diffusion Blocking Layer and its Impact on the Performance of Perovskite Photovoltaics. *ACS. Appl. El. Mat*, 5 (10), 2023]. The scope of our current work in the LUMINOSITY project includes the fabrication of PSCs using large scale industrially compatible techniques. The incorporation of diffusion blocking buffer layers as a viable strategy to improve the roll roll-to-roll printed PSCs will be discussed.

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Topic preference: Materials for Energy
Presentation preference (oral/poster): Oral
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Improving Lifetime of Methylammonium-Free Perovskite Solar Cells Through Additive Engineering

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Abstract: Instability of Perovskite solar cells (PVSCs) is an established key challenge for the commercialization of this technology due to high moisture sensitivity of perovskite film. Additive engineering is a strategy to enhance the performance and stability of PVSCs.[1] In this presentation, we show that the addition of nitrobenzene in the perovskite precursor solution yields PCE of around 18 % for small scale methylammonium-free ($FA_{0.83}Cs_{0.17}Pb(I_{0.83}Br_{0.17})_3$ PVSC with improved PCE reliability and air/humidity degradation resistance. Nitrobenzene based PVSCs retain over 85% of their initial mean PCE after 1500 h in air, with the additive-free PVSCs degrading more than 65% in the same time span. Photocurrent mapping under accelerated humidity test (75% RH) reveals that the addition of nitrobenzene mitigates the degradation of perovskite film leading to more stable PVSCs.[2] Within the LUMINOSITY project, large-scale and industrially compatible methods are applied for the development of PVSCs.[3] By incorporation of additives in the precursor perovskite solution we have developed meniscus coating PVSC under ambient conditions (40 - 50 %RH) with PCE up to 13.3% so far.

Acknowledgements: This project has received funding from the European Union’s Horizon Europe Research and Innovation Programme under grant agreement No 101147653 (project LUMINOSITY).

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Topic preference: Materials for Energy
Presentation preference (oral/poster): Oral
Full name of presenting author: Sophia C. Hayes
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Temperature dependent structural evolution of an organic donor-acceptor polymeric semiconductor

S. C. Hayes, A. Kyrri, E. Lariou

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Abstract: Significant leaps in power conversion efficiencies (PCE) have been achieved in OPVs thanks to the combination of low-bandgap donor-acceptor polymers with non-fullerene acceptors, surpassing 19%. This study focuses on a donor-acceptor polymer known as PCE11 (poly[(5,6-difluoro-2,1,3-benzothiadiazol-4,7-diyl)-alt-(3,3´´´-di(2-octyldodecyl)2,2´;5´,2´´;5´´,2´´´-quaterthiophen-5,5´´´-diyl)]), that shows highly tunable optical properties under various processing conditions and a reported PCE of 11.5%.[1] Temperature-dependent absorption measurements showed a slight red shift and a clear vibronic structure upon cooling, similar to other donor-acceptor polymers in the literature,[2] usually interpreted as increase in backbone planarity and consequently conjugation length, but with no structural data to support this assumption. Here, we employ temperature-dependent Resonance Raman (RR) spectroscopy to develop a basic understanding of how temperature affects the polymer conformation and thus its optoelectronic properties. We find, contrary to the interpretation of temperature-dependent absorption spectra, increase in the polymer backbone torsional disorder when cooling, attested by upshifts in the thiophene and benzothiadazole C=C stretches and changes in the relative intensity between the various vibrational bands, which is supported by DFT calculations. These results suggest that interpretation of the optical spectra is not as simple as described in the literature so far, but a combination of structural information from RR and excitonic models for photophysical aggregates is necessary to understand the optical properties. Interestingly, the RR data suggest a phase transition around 200 K that could be responsible for the modification of excitonic coupling, through reduction of the contribution of inter chain coupling, explaining thus the increase in the 0-0 band with cooling, as expected for J-aggregates.

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Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Nanostructured Plasmonic Sensors for Chemical Monitoring via Surface Enhanced Raman Spectroscopy

Chrysafis Andreou

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Abstract: Despite their inconceivably small size, molecules in our environment, food, and body have a tremendous impact on our health, safety, and well-being. The ability to detect and identify molecules of interest in a variety of samples efficiently and effectively can lead to better chemical screening and monitoring. Surface enhanced Raman spectroscopy (SERS) has been established as an exquisitely sensitive and specific molecular sensing technique – molecular vibrations allow fingerprint-like identification of the molecule and plasmonic enhancement allows detection with down to single-molecule sensitivity. Plasmonic nanostructures can be fabricated via either uncontrolled aggregation of colloidal nanoparticles (bottom-up) or high-precision nanofabrication (top-down). To date, the technique has been limited to single timepoint applications, as these substrates are not amenable to regeneration and reuse. Recently, we have developed methodologies that allow dynamic monitoring of fluid flows via SERS via timeseries analysis. By combining microfluidic flows and plasmonic substrates we have been able to detect different analytes in aqueous samples, in a quantitative and dynamic way. Our dynamic monitoring technique has been applied to colloidal substrates as well as to nanostructured surfaces grown in situ. Model small molecule analytes, as well as acrylamide, a common food contaminant, have been detected in this way. This research can lead to applications in monitoring of environmental, industrial, and other processes.

Topic preference: Materials for Energy
Presentation preference (oral/poster): Oral
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Routine operando studies with Near Ambient Pressure (NAP) - XPS

Liana Socaciu-Siebert

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Abstract: Over the last decades it has been possible to develop XPS systems that can work far beyond the standard conditions of high or ultrahigh vacuum. Thus, Near Ambient Pressure (NAP) - XPS has become a rapidly growing field and has demonstrated its capability in a wide variety of applications. Starting from operando studies of surface reactions in catalysis, the applications soon have been extended towards studies of processes at liquid surfaces. Since more than 15 years, the need for basic studies of the fundamental chemistry at solid-liquid interfaces has attracted growing interest. Dip-and-pull experiments at synchrotrons finally demonstrated, that in-situ and operando XPS in electrochemical experiments can be realized, significantly contributing to the basic understanding of modern energy converting or storing devices, like batteries, fuel cells, etc.

The development of pure laboratory NAP-XPS systems by using small spot and high photon flux density monochromatic X-ray sources together with the development of optimized sample environments, like Peltier coolers and operando electrochemical cells open the possibility for the preparation and analysis of a multitude of liquid samples or solid-liquid interfaces on a reliable daily base. Furthermore, the combination of various analysis methods (NAP-SPM, IRRAS, NAP-HAXPES etc.) allows for gaining insights into the fundamental processes that take place during a chemical reaction.

Existing solutions for NAP-XPS will be presented, with an emphasis on latest developments of instruments and material analysis methods. Examples and results will be shown as well as future perspective of applications and scientific contributions of routine operando NAP-XPS.

TUESDAY 16 SEPTEMBER 2025

TALKS – SESSION 2

Topic preference: Advance Functional Materials
Presentation preference (oral/poster): Invited Talk
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Tailoring solid state nanopores via computational modelling

P. Wei, M. Kansari, L. Li, P. Campen, C.K. Das, M. Fyta

Computational Biotechnology, RWTH Aachen University, Worringerweg 3, 52074 Aachen, Germany

Abstract: Solid state nanopores are nanometer-sized openings in materials of different types and thicknesses. These can electrophoretically drive charged (bio)molecules by means of an applied voltage difference. The transport of the analytes is strongly dependent on the interplay of the electrophoretic and the electroosmotic forces generated within the nanopores and gives rise to measurable ionic and/or electronic currents along and across the pores. Using computer simulations at diverse spatiotemporal scales, we model the transport of different analytes, such as single and molecular ions, DNA molecules and short peptides though solid state nanopores. For the latter, we probe 2D materials, such as graphene and molybdenum disulfide, as well as novel Janus type materials. The simulations allow us to obtain a detailed atomistic insight into the exact interactions of the nanopore material, the analyte, and the surrounding liquid environment. We discuss these insights in the concept of DNA sequencing, detection of post-translational modifications in proteins, desalination and blue energy generation.

Topic preference: Advance Functional Materials
Presentation preference (oral/poster): Invited Talk
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Data-Driven Electronic Structure Calculations at Finite Temperature

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Abstract: The role of data in modern materials science becomes more valuable and accurate when effects such as electron-phonon coupling and anharmonicity are included, providing a more realistic representation of finite-temperature material behavior. Furthermore, positional polymorphism, characterized by local atomic disorder beyond the reach of standard diffraction techniques, is a critical yet underexplored factor in understanding the electronic structure and transport properties of energy-efficient materials. In this talk, I will present a novel first-principles methodology for polymorphous materials [1,2], rooted in the special displacement method [1,2,3], that offers a systematic and alternative approach to molecular dynamics (MD) for exploring finite-temperature properties. By enabling a unified and efficient treatment of anharmonic lattice dynamics, electron-phonon coupling, and positional polymorphism, our approach generates essential data to predict temperature-dependent band gaps, effective masses, phonon dynamics, free energies, and charge carrier mobilities [4,5,6,7]. Designed with a high-throughput spirit, this framework has been applied across a range of halide perovskites, systematically uncovering trends and insights into their thermal and electronic behaviors. Our methodology bridges theoretical and experimental insights [4,5,6,7] while aligning with the paradigm of data-driven materials discovery, where computation and experimentation converge.

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Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Deep Neural Networks for Predicting the Mechanical Properties of Glassy Polymer Nanocomposites

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Abstract: Creating innovative materials with superior properties has been a core engineering challenge since the early days of science. Within this context, modeling and testing rationally designed polymer based nanocomposites (PNCs) is an emerging field that can yield novel materials with superior mechanical properties and added functionalities [1]. Here we propose a computational methodology for predicting the distribution of the mechanical properties in atomistic polymer-based nanostructured systems. The use of atomistic simulations is key in unravelling the fundamental mechanical behavior of composite materials. Most simulations involving the mechanical properties of PNCs concern their global (average) properties, which are typically extracted by applying macroscopic strain on the boundaries of the simulation box and calculating the total (global) stress by invoking the Virial formalism over all atoms within the simulation box; hence, extracting the pertinent mechanical properties from the corresponding stress-strain relation [2-3]. However, in order to probe the distribution of mechanical properties within heterogeneous multi-component polymer-based systems, a detailed computation of stress and strain fields for each atom within the simulation box is necessary, as shown recently by H. Reda et al. [4]. Starting from a recent work, we introduce a Machine Learning (ML) approach to probe the distribution of mechanical properties in heterogeneous glass polymer nanocomposites by directly computing the stress and strain at the atomic level, and averaging over all atoms within the simulation box to compute the global strain. With ML we train a U-net based network, which takes as input information about every atom in the system and predicts their corresponding stress and strain. The proposed ML tool eliminates the complexity of using complicated physical based relations, while managing to reduce the computation time by several orders of magnitude.

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Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Active Learning of Atomic Size Gas/Solid Potential Energy Surfaces via Physics Aware Models

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Abstract: Sensing gas pollutants at the nanoscale is a complex challenge. Molecular Dynamics (MD) simulations can offer valuable insights for designing nanosensing devices, but their reliability depends heavily on the accuracy of the underlying force field (FF), which governs atomistic interactions. To address this, we propose a generic active learning (AL) framework for developing accurate, physics-aware FFs for nanostructured systems involving atomic-sized metal clusters and gaseous air pollutants-critical for advancing environmental sensing technologies. The AL framework iteratively refines FFs using ab-initio Density Functional Theory (DFT) data. Candidate structures are generated via stochastic methods (e.g., Monte Carlo or Langevin dynamics), and a subset is selected for DFT labeling and FF performance evaluation. These data are then used to retrain the FF in the next iteration. This self-improving loop enables efficient exploration of the relevant configurational space. The framework is broadly applicable, producing FFs that capture diverse interaction types, including cohesive, physisorption, and chemisorption forces, within silver nanoclusters and gas/cluster hybrids.[1] The resulting models use physically meaningful descriptors and flexible potential terms, achieving a balance between accuracy, efficiency, and transferability. Prediction performance is comparable to ab-initio calculations and modern machine learning models, yet computationally efficient like semi-empirical potentials, making this approach a promising tool for simulating complex gas–solid interfaces.[2]

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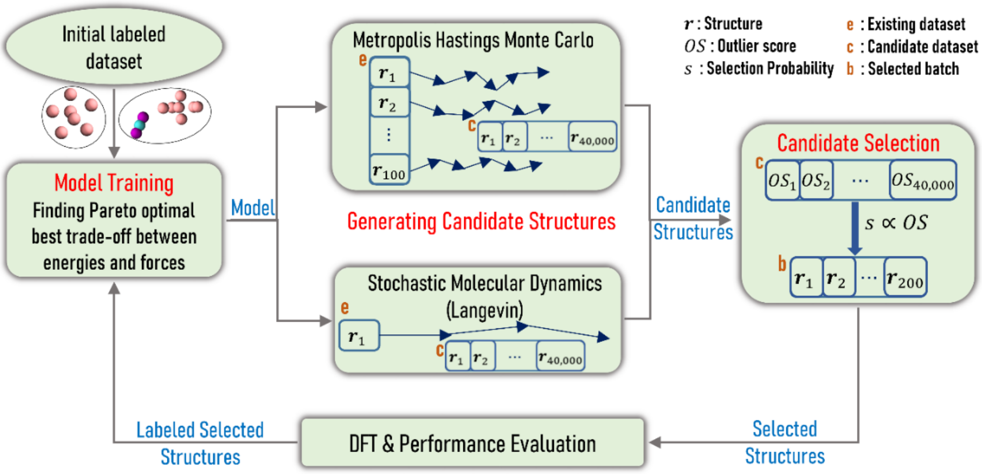

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Computational inverse homogenization approach for predicting the mechanical properties of randomly distributed ellipsoidal inclusions of composite materials

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Keywords: inverse methods, homogenization, polymer nanocomposites, in-silico materials design, biochar-polymer composites, circular nanocomposites, circular materials

Abstract: Designing the next generation of circular materials requires a comprehensive understanding of their mechanical performance. Here, we present a computational framework for the in-silico design and optimization of AgReCOMPOSITES—sustainable, circular materials derived from recycled plastic and biochar produced from agricultural and livestock waste. This framework combines hierarchical homogenization and Finite Element Methods with experimental data to predict the mechanical performance of biochar-polymer composites, enabling the optimization of mixing ratios and geometrical configurations for superior functionality. A key focus is on the random distribution of the ellipsoidal nanoparticle reinforcements—which significantly influences the mechanical response of the composite material. In this work we developed an inverse numerical homogenization model that predicts the inclusions properties with excellent agreement to experimental data. We extend these methodologies to AgReCOMPOSITES, showcasing the potential and challenges of the computational inverse homogenization methodology in transforming sustainable, circular materials design.

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Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Modelling of the shear-induced migration of rigid and deformable particles in Newtonian and non-Newtonian fluids

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Abstract: Shear-induced migration is a key phenomenon in suspension flows, since particles tend to migrate from areas of high shear stress to areas of low shear stress [1], [2]. We investigate shear-induced migration of rigid and deformable particles suspended in Newtonian and non-Newtonian fluids by extending the constitutive model proposed by Phillips et al. [3], which considers particle migration due to gradients in viscosity and concentration of rigid spheres in a Newtonian suspending fluid, in Couette and Poiseuille flows. We introduce the particle deformability parameter λ to account for the deformability of particles, which is a ratio between the internal and the external viscosities. We observe the effect of particle deformability, average volume fraction, and ratio of two transport phenomena (diffusion and convection) on the particle distribution and the velocity profiles. Furthermore, we provide a comparison with experimental and DPD simulation data. Since the impact of particle deformability in shear-induced migration is still unclear, our work fills this gap and allows for further future generalizations, e.g., by including the RBCs-plasma interactions occurring in micro vessels.

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Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Oral
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Modeling the Rheological Behavior of Cement Pastes over a spectrum of temperature and water-to-cement ratio

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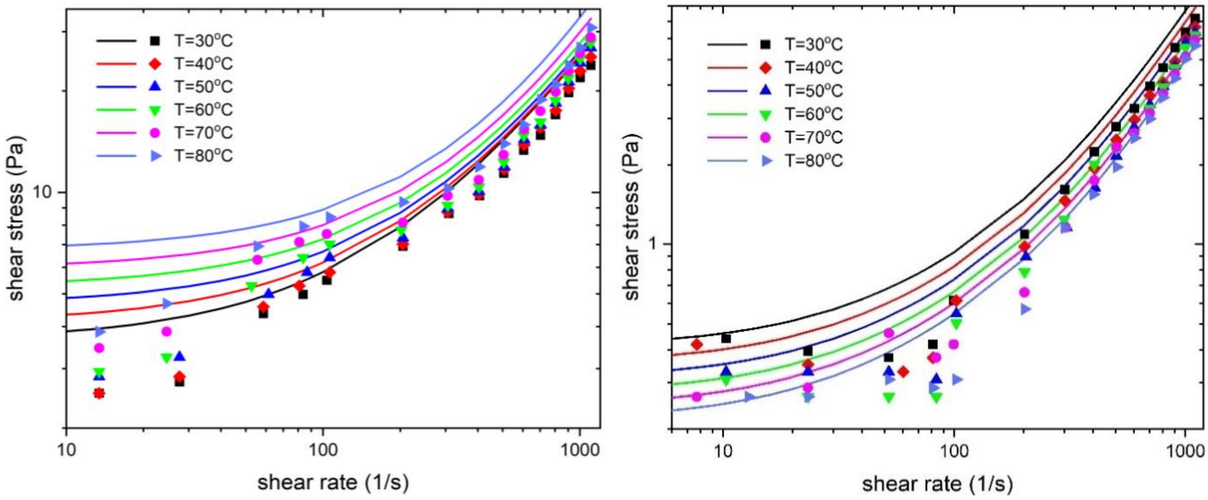
Abstract: In the construction industry, cement, alongside other materials such as gravel, sand, and lime, is one of the most necessary building materials. A carefully performed extensive analysis of the dual, reversible and irreversible, rheological behaviour of cement pastes is paramount for the effective and appropriate use of cement as a building material. When mixing cement with water, a suspension is created at early times which due to agglomeration forms a reversible structure, whereas the hydration reactions between cement particles and water have an important effect at later times; it is this irreversible structure that eventually leads to the solidification of the cement paste. In the present work, we use our own recently proposed constitutive rheological model for predicting the rheological response of the cement paste, which is by construction compatible with the laws of non-equilibrium thermodynamics and expand its use to cover a vast spectrum of temperature and water-to-cement (w/c) ratios. We provide a thorough comparison of the model's predictive capacity by comparing it with available experimental data (see Fig. below). It is expected that the use of the fully parametrized model will enable the execution of numerical simulations to elaborate the importance of cement paste rheology in actual pumping operations, and open the way to describe the rheological characterization of mortars (cement paste plus sand particles) and concrete (mortar plus gravel particles).



Left: w/c=0.7, Right: w/c=2

TUESDAY 16 SEPTEMBER 2025

TALKS – SESSION 3

Topic preference: Micro/Nano Electronics
Presentation preference (oral/poster): Oral
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Computational Study of Mixed Dislocations in GaN: Energetic Stability and Environmental Effects

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Abstract: Group-III nitrides are key materials for optoelectronic and power electronic applications. However, dislocations constitute a longstanding and controversial topic in the field of III-Nitride materials. These defects have recently re-attracted the interest of the III-Nitrides community due to their alleged detrimental effects on the properties and efficiency of power-electronic devices such being the root cause of device leakage and breakdown. Recently it has been shown that C segregation at dislocations in GaN correlates strongly with the electrical activity of these defects, highlighting the critical role of dislocation-impurity interactions in device behavior [J. Appl. Phys. 136, 045704 (2024)]. Understanding the atomistic mechanisms that govern dislocation stability in GaN is crucial for optimizing the performance and reliability of modern power electronic devices.

In this work, we investigate various mixed dislocations in GaN using density functional theory calculations, aiming to assess their properties (energetics, atomic and electronic structure) under different growth conditions. To model dislocations, clusters consisting of ≈1000 atoms with hexagonal cross section and a single defect have been constructed. In total more than 200 different core structures have been considered.

Based on these calculations a phase diagram was constructed, revealing the energetically favorable cores under different growth conditions. Notably, hollow/open cores passivated with H or NHx molecules show enhanced stability under N-rich and H-rich conditions. Under extremely H poor, as it is relevant for MBE growth, stoichiometric and metallic cores are energetically favorable under N-rich and G-rich conditions, respectively. Based on the aforementioned, we will further discuss potential implications of the strain field and the open core formation on the impurities' diffusion and segregation and the properties and the efficiency electronic devices.

Acknowledgements: This work was supported by the ALL2GaN Project (Grant Agreement No 101111890) through the Chips Joint Undertaking and its members, including the top-up funding by Austria, Belgium, Czech Republic, Denmark, Germany, Greece, The Netherlands, Norway, Slovakia, Spain, Sweden and Switzerland.

Topic preference: Micro/Nano Electronics
Presentation preference (oral/poster): Oral
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Tunable Optoelectronic Neuromorphic Behaviour in MoS_2 Memristors with Pt Nanoparticle Decoration for Energy-Efficient Spiking Neural Networks

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Abstract: The optoelectronic neuromorphic characteristics of MoS_2 present a promising avenue for the advancement of neuromorphic computing systems that emulate the behaviour of biological neural networks. Key features such as memristive effects and photo-synaptic responses enable diverse mechanisms for mimicking both synaptic and neuronal functions.

In this context, we fabricated a forming-free memory device based on a monolayer of MoS_2 (~100 μm in size) grown using Chemical Vapour Deposition (CVD) [1] decorated with small platinum (Pt) nanoparticles (NPs) approximately 3 nm in diameter. The NPs were fabricated in vacuum using a cluster beam synthesis method [2]. The influence of Pt NP surface density on the device's optoelectronic neuromorphic behaviour under ultraviolet illumination (λ = 390 nm) was systematically examined.

Reference devices without Pt NPs exhibited only synaptic behaviour, while those with a moderate NP density demonstrated neuron-like spiking responses. At a higher density, the spike frequency was reduced. A variety of synaptic plasticity and neuronal coding behaviours were experimentally observed [3].

These phenomena are attributed to band bending at the Pt NP–MoS_2 interface, causing electron trapping [2] on the metallic NPs—a process confirmed by photoluminescence quenching—followed by a subsequent de-trapping process. This functional diversity enabled the implementation of a fully optoelectronic spiking neural network.

Given the low energy required per spike (~400 pJ), the device achieved a significantly reduced power consumption of approximately 320 μW during optical image pattern recognition. This work offers critical insights into the emulation of artificial synaptic and neuronal behaviour and highlights the potential of developing next-generation, fully memristive artificial neural networks with ultra-low energy demands.

The research was supported by EU-project ELEGANCE (No 101161114).

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Topic preference: Micro/Nano Electronics
Presentation preference (oral/poster): Oral
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Optical profilometry for 3D mapping of Photonic Integrated Circuits

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Abstract: Optical techniques for surface topography measurements have become crucial in microelectronics and photonics for real-time monitoring of surfaces covering areas of a few microns to millimetres. In particular, step heights in the order of nm created by means of lithography, relative to the underlying layers of the chip, should be measured because it is paramount to the performance of the microelectronic or photonic device. Among these methods, phase shifting interferometry (PSI), a technique based on light interference, stands out as a non-contact technique, used to determine height differences between neighbouring areas. This study presents a miniaturized Michelson-type optical profilometer, which is able to measure patterned electrodes and waveguides on silicon wafers. The system consists of a laser source that serves both as the illumination and coherent light source for fringe formation (in particular, on-axis single fringe formation) a 50x magnification 4F telecentric system and a beam splitter alongside an independent reference mirror mounted on a piezoelectric actuator. The height information is processed using the 13-step Phase Shifting Algorithm (PSA). The current configuration achieves accurate step height measurements of at least 20nm, with a lateral resolution of approximately 2μm and a field of view of 0.27 × 0.18mm². Photographs / graphics may be used if necessary to substantiate results.

Topic preference: Micro/Nano Electronics
Presentation preference (oral/poster): Oral
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The Impact of Hole Transport Layers on Charge Transport and Efficiency in Organic Electronic Devices.

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Abstract: Solution-processable Organic Electronic Devices, such as OPVs and OLEDs, possess great potential for flexible and large-area electronic applications. However, their up-scaling fabrication, particularly through Roll-to-Roll manufacturing processes, remains a great challenge up to this day. A key factor, among others, that determines the performance of the device is the controlled and efficient transport of charge carriers across device interfaces. Imbalanced transportation can cause carriers to accumulate and become trapped at the interfaces between the functional layers of the device. Following this, the accumulation of carriers is influenced and determined to a large extent by internal factors such as energy-level alignment as well as the quality of the interlayers formed during the deposition process of the multi-stack device. Toward this direction, in our study, three different Hole Transport Materials, including Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), Poly(9,9-dioctylfluorene- alt-N(4-sec-butylphenyl)-diphenylamine (TFB) and Copper(I) thiocyanate (CuSCN), were deposited as thin films and systematically characterized in terms of their optical, electrochemical, morphological, and photophysical properties, using various experimental techniques. A comparative analysis was conducted to evaluate how these HTLs influence the charge injection efficiency, based on their energy-level alignment, and interfacial morphology. The methodology developed in this study is demonstrated through its application in organic electronic devices. The findings highlight the importance of of energy-level alignment and interface quality at the operation of the fabricated devices.

Acknowledgements: This work has been supported by the projects: “Development of efficient third generation PV materials and devices to enhance the competitiveness of the productive sector in green energy" (3GPV-4INDUSTRY) (TAEDR code 0537347) and the Horizon Europe COPE-Nano (GA 101059828)

Topic preference: Materials for Energy
Presentation preference (oral/poster): Oral
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Silicide thermoelectric modules based on high purity Si and recycled Si-kerf

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Abstract: Thermoelectric energy conversion devices utilizing non-toxic, sustainable, and cost-effective silicide compounds hold significant promise in the context of the green energy transition. This promise is further enhanced by incorporating recycled silicon kerf waste—a byproduct of the PV industry—within a circular economy framework.

This work describes the development of thermoelectric modules for power generation, based on n-type magnesium silicide and p-type manganese silicide synthesized from high purity Si (commercially available) and recycled Si-kerf from the PV industry.

Metallization based on sputtered Ni/Cu bilayers and specific contact resistance analysis are performed to evaluate the aptness of the metallization and bonding methodologies, through the transfer length- and the scanning probe- methods respectively. Deposition conditions are optimized, and a reduction of the metallization-related contact resistance is achieved. Improvement of silver sintering bonding is enabled through the increase of the thermoelectric legs surface roughness, which is accompanied by lower cumulative specific contact resistance values.

Fabrication of 4-leg thermoelectric modules, serving as proof-of-concept prototypes for the recycling of Si-kerf, is shown, and good agreement between experimental and simulated (COMSOL Multiphysics®) performance is obtained. Upscaling from 4-leg proof-of-concept prototypes to larger 16-leg Si-kerf based modules is also achieved, with high power densities being demonstrated as well.

As such, development and upscaling of high-performance silicide TEMs based on high purity- and recycled Si is achieved and signals the potential in upcycling of Si-kerf waste material.

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Topic preference: Soft Condensed Matter
Presentation preference (oral/poster): Oral
Full name of presenting author: Stefanos Basim Atata
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A Comparative Study on the Effect of Nanoparticle Geometry on the Nematic Phases of a Bimesogenic Liquid Crystal

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Abstract: Nematic liquid crystals (NLCs) are self-organized, anisotropic nanomaterials widely used in liquid crystal display (LCD) technology. The dispersion of nanoparticles (NPs) into NLC systems aims to enhance their physical and chemical properties. Key factors influencing the behavior of such nanocomposites include the shape, size, and chemical composition of the NPs. Among nematic liquid crystalline mesophases, the twist-bend nematic (N_{tb}) phase is characterized by a doubly degenerate helical structure formed by achiral molecules. While liquid crystal–liquid crystal mixtures exhibiting the N_{tb} phase have been extensively studied, corresponding research on liquid crystal–nanoparticle nanocomposites remains limited.

We present a comparative investigation of the impact of spherical, rod-like, and disk-like NPs on the electrooptical properties of a liquid crystal exhibiting both uniaxial nematic (N_u) and N_{tb} phases. Three series of nanocomposites were prepared, each consisting of the mesogenic dimer 1'',9''-bis(4-cyanobiphenyl-4'-yl)nonane (CB9CB) doped with, respectively, CdSe/ZnS quantum dots, hydroxyapatite nanorods, and $CuFeS_2$ nanoplatelets. The uniformity of NP dispersion within the CB9CB microstructure, as well as the thermal behavior of the mesophases, was investigated via polarized optical microscopy. Phase diagrams of the nanocomposites were constructed as functions of temperature (T) and NP mass fraction (χ). The influence of NPs on the nematic optical alignment and the conical tilt angle of the heliconical structure was analyzed. Additionally, the voltage threshold of both nematic phases and the switching times of the N_u phase were measured under the influence of an external electric field as functions T and χ.

WEDNESDAY 17 SEPTEMBER 2025

TALKS – SESSION 1

Topic preference: Advance Functional Materials
Presentation preference (oral/poster): Invited Talk
Full name of presenting author: Spyros Kassavetis
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Alternative Plasmonic Nanomaterials and Fabrication Processes

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Abstract: Transition metals nitrides (TMNs) emerge as alternative plasmonic nanomaterials suitable for a wide range of applications from photovoltaics to photonics and medicine, as they combine substantial electronic conductivity, high melting point (>3000 K), tunable work function, and stability in hostile chemical environments.

In this work, we present the plasmonic properties of TMNs as well as the use of cost-efficient processes for the fabrication of plasmonic TMNs either on surfaces or in solvents (colloidal plasmonic nanoparticles NPs). We focus on Titanium Nitride (TiN), the archetypical TMN, and we fabricate high crystalline quality TiN nanostructures with controlled spacing, tunable dimensions (thickness and lateral) and shape (nanotriangles, nanorods, nanorod rings, and nanowires), using a combination of Nanosphere Lithography (NSL) and several reactive magnetron sputtering (MS) deposition processes such as DC, Closed-Field Unbalanced MS and Highly Power Impulse MS (HIPMS) with the aim to study the fundamentals that unlock the fabrication of high quality TMNs nanostructures for plasmonic applications. NSL appears as a very promising approach, with rapid implementation and compatibility with wafer-scale processes, combines the advantages of both top-down and bottom-up approaches and includes: (a) development of the nanospheres monolayer colloidal mask, (b) deposition of the desired material in the empty space between the nanospheres and (c) removal/lift-off of the nanosphere colloidal mask to “reveal” the highly ordered nanostructures.

Finally, we present and discuss the use of short and ultra-short laser beam processes for the fabrication of high quality TiN NPs in solvents, with the target to promote the applications of TMNs in printed electronics and medicine.

Acknowledgements: S. Kassavetis is supported by “Development of efficient third generation PV materials and devices to enhance the competitiveness of the productive sector in green energy" (3GPV-4INDUSTRY) (TAEDR code 0537347) and the Horizon Europe COPE-Nano (GA 101059828). Horizon Europe COPE-Nano (GA 101059828) Projects.

Topic preference: Photonics and Optoelectronics
Presentation preference (oral/poster): Oral
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Spectral reflectivity calculations of Fiber Bragg Gratings (FBGs) with intensity-depended refractive index

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Abstract: Germano-silicate glass fibres for telecom applications have been extensively studied in the past for their core's refractive index nonlinearity n_2, and found to be in the order of 10^{-20} m^2/W for 1.55μ. Although this magnitude may be enhanced by increasing the concentration of GeO_2 within the core, the non-resonant nonlinearity remains low. Nevertheless, high-power fibre applications -such as fibre laser configurations- often incorporate FBGs for a specific wavelength operation. Erbium-doped ring fibre laser topologies, utilize FBGs for wavelength selection, thereby requiring the management of elevated optical intensities within the fibre core. Furthermore, materials and glasses, such as the chalcogenide glasses with significantly higher nonlinearities, may be alternatives for high-power fibre applications, while the inscription of gratings in their core may be implemented by direct-inscription techniques. A potential interest may arise from the combination of strong nonlinear host fibre core, together with a grating inscription that accepts high optical intensities. Particularly, nonlinear phenomena in the optical waveguiding structures have been shown promising, although complicated, while they opened new optical fibre applications. Furthermore, the operation of an FBG under strong nonlinear conditions, may introduce notable effects that either alter their linear response or offer advantages for specific device applications.

The present work is motivated by these considerations and aims to study the spectral reflectivity of an FBG with nonlinear fibre core index. The calculations herein, do not focus on a specific material, inscription or application, however, they may reveal the potential new characteristics from two combined mechanisms; the intensity-dependent index nonlinearity and the accumulated interference at the input port of a grating.

The simulation framework is based on the Coupled-Mode-Theory, implemented via either the Transfer Matrix or the Transmission Line Method in their discrete form. Both methods' calculation techniques are adapted and modified to incorporate nonlinear index variations through linear and uniform segmentation.

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Topic preference: Photonics and Optoelectronics
Presentation preference (oral/poster): Oral
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Slow-light enhanced integrated plasmo-photonic index sensor

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Abstract: We investigate the theoretical performance limits of an integrated plasmo-photonic Mach-Zehnder interferometer (MZI) enhanced by the slow-light effects of Bragg gratings. We develop and validate a convenient one-dimensional effective model of the structure and use it to systematically explore the design parameters of Bragg-defined coupled cavity structures decorating the plasmonic strip sensor. We consider their photonic band structure, slow-light properties, and overall sensitivity enhancement. Substantial sensitivity improvements over the corresponding pure plasmonic systems are found, exceeding 10^5 nm/RIU at the photonic bandgap edges and at the coupled cavity bands. Practical considerations, such as free-space scattering and fabrication constraints are addressed, with higher order Bragg gratings proposed as mitigation. This work provides a comprehensive framework for optimizing slow-light plasmo-photonic sensors, highlighting their potential for biological and chemical sensing application.

Acknowledgments: This work was supported by the EU H2020 RIA under grant agreement 101093166 (AMBROSIA).

Topic preference: Photonics and Optoelectronics
Presentation preference (oral/poster): Oral
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Structural and optical properties of zinc oxysulfide semiconductor thin films

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Abstract: Zinc Sulfide (ZnS) and Zinc Oxide (ZnO) are wide band gap II-VI semiconductor materials with excellent optical transparency, chemical stability, and high refractive indices, making them attractive for a plethora of applications in optoelectronic devices, photodetectors, and light-emitting diodes (LEDs). In this study, thin films of pure ZnS, ZnO, and solid solutions of $ZnO_{1-x}S_x$ were deposited on silicon wafers and glass substrates using electron beam (e-beam) evaporation under high vacuum conditions. For the deposition, compressed pellets from high purity ZnO and ZnS powders were used in variable weight compositions. The structural properties of films were characterized using X-ray diffraction (XRD), which revealed that pure ZnS and ZnO films exhibited polycrystalline behaviour with cubic (zinc blende) and hexagonal (wurtzite) phases, respectively, while the films with intermediate target composition were amorphous. X-ray reflectivity (XRR) was employed to determine film thickness, density, and surface/interface roughness, confirming smooth, uniform growth across all samples. Optical properties were evaluated using UV-Vis spectroscopy in both transmittance and reflectance modes. All films demonstrated high transmittance in the visible spectral region, exhibiting bandgaps from 3.4 eV to 3.9 eV. These findings indicate that e-beam evaporation is an effective technique for fabricating high-quality thin films with tunable structural and optical properties.

Topic preference: Photonics and Optoelectronics
Presentation preference (oral/poster): Oral
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Molecular Polaritonics: Controlling photochemistry with quantum optics

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Abstract: Molecular polaritonics involve the strong coupling of molecular materials to confined optical fields, and the formation of new hybrid polariton states that are a linear superposition between excitons and photons. In the recent years, polaritons have become a platform to study fundamental and intriguing phenomenology at room-temperature; a few realisations among many include Bose-Einstein condensation, access to topological physics and ultralong-range energy transfer. It has been recently shown that the excited-state reactivity of molecular materials could also be altered in polaritonic systems [1]. One of the most fundamental photophysical reactions in molecular materials is photobleaching. This is particularly important in organic optoelectronic devices because it can cause permanent damage on the devices and limit their operational performance and stability. In recent studies, it was shown that the photobleaching could be suppressed in dye-coated plasmonic nano-structures [2] as well as microcavities filled with P3HT molecules [3] when compared with control films. Here, we introduce a new microcavity design that allowed the observation and quantification of the photobleaching effect. A shown in Figure 1. we have used the Transfer Matrix Method (TMM) to design and fabricate a series of multilayered optical microcavities containing a combination of the J-aggregated dye TDBC and SiO_2 spacer layers. Following careful design of the multiple layer thicknesses of the microcavities, we have been able to realize structures that operate in either the weak or strong coupling regime while maintaining similar design characteristics. Most importantly, the thickness of the active molecular layer used is a few tens of nm allowing the entire number of molecules to either reside at the node or anti-node of the confined electric field, rather than being distributed along the total volume of the microcavity. Using this approach, we can maximise or fully suppress the cavity effects depending on the selected design.

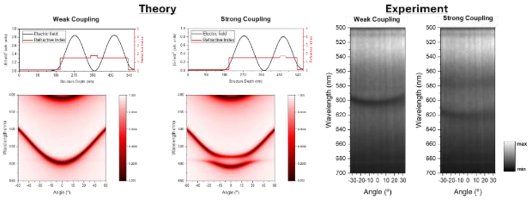

Figure 1. Theoretical design of weakly and strongly coupled microcavities showing angle-resolved white-light reflectivity along with the refractive indices and the distribution of the E-field as a function of cavity depth (left panels). Experimental angle-resolved white-light reflectivity results of the fabricated weakly and strongly coupled microcavities (right panels).

Microcavities have been studied using a k-space imaging technique measuring white-light reflectivity and photoluminescence, with the data being fitted with a standard coupled oscillator model to allow light-matter interaction parameters to be extracted. Next, we have studied the photostability of weakly and strongly coupled microcavities as well as non-cavity control films, through photoluminescence measurements. Following extended laser excitation, we observed a suppression of the photobleaching process in strongly coupled microcavities as compared to weakly coupled structures and non-cavity control films.

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Topic preference: Photonics and Optoelectronics
Presentation preference (oral/poster): Oral
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Surface-Enhanced Raman Scattering Coupled with Chemometrics for Advanced Food Safety Monitoring

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Abstract: Surface-Enhanced Raman Scattering (SERS) has emerged as a powerful analytical technique for rapid, sensitive, and non-destructive detection of chemical contaminants in food. Our target is to establish a robust methodology that combines novel SERS nanomaterials with chemometrics for enhanced food safety monitoring, with the first application focused on detecting and quantifying acrylamide, a known carcinogen formed during high-temperature processing of carbohydrate-rich foods, using gold-nanoparticle decorated titanium dioxide nanowires.

Acrylamide contamination in processed foods such as potato chips, bread, and coffee poses a significant public health concern. Current detection methods, although accurate, often require extensive sample preparation, long analysis times, and expensive instrumentation. In contrast, SERS offers the potential for rapid, low-volume analysis with high sensitivity and specificity. We employ engineered SERS substrates combining metallic nanoparticles and nanowires, self-assembled in a layer via dielectrophoresis, to achieve high analytical performance, maximizing Raman signal enhancement through synergistic plasmonic effects. This hybrid nanostructure design significantly amplifies the Raman scattering of analyte molecules, enabling ultra-sensitive detection directly in complex food matrices. The integration of chemometric approaches allows treatment of spectroscopic measurements, thus enhancing the reliability and interpretability of complex spectral data.

This novel approach aims to deliver a portable, cost-effective, and user-friendly tool for real-time food safety assessment, with applications spanning from research laboratories to industrial quality control settings and regulatory agencies, as well as the development of next-generation sensing platforms for safer and more transparent food systems.

WEDNESDAY 17 SEPTEMBER 2025

TALKS – SESSION 2

Topic preference: Soft Condensed Matter
Presentation preference (oral/poster): Invited Talk
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Use of non-equilibrium thermodynamics to derive a constitutive rheological model with a variable entanglement density

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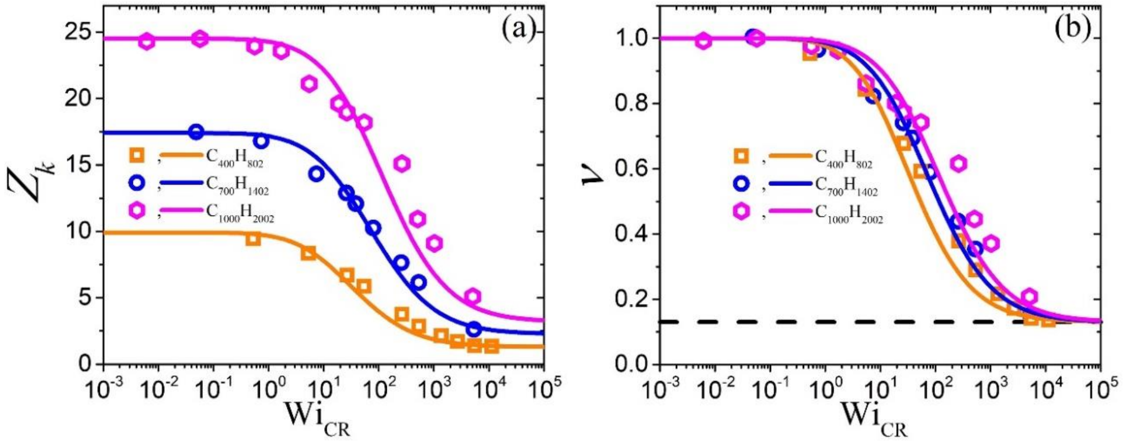
Abstract: Detailed nonequilibrium molecular dynamics (NEMD) simulations have shown that under flow, there is a strong reduction in the average number of entanglements per chain, a mechanism known as convective constraint release (CCR) [1,2]. Initially Ianniruberto and Marrucci [3], and more recently Dolata and Olmsted [4], proposed new theoretical models that account explicitly for flow-induced disentanglement. In this work, we employ the single-generator bracket formalism of nonequilibrium thermodynamics by Beris-Edwards [5] to derive a similar constitutive model [6]. In the new approach, entanglement destruction is obtained by coupling the entanglement density directly with the velocity gradient and not with the orientation tensor. Direct comparison with NEMD simulation data, as shown in the figure below, shows that the model can accurately describe the loss of entanglements due to the applied flow for three molecular weights by using the same value for the CCR parameter and the viscometric functions, although some discrepancies are observed in the description of the second normal stress coefficient. Overall, the model proposed here is carefully derived via NET and builds upon, the work of Ianniruberto-Marrucci and Dolata-Olmsted when stretching is not considered.



Comparison of model predictions (lines) with the NEMD simulation data (symbols) of Nafar Sefiddashti et al. [2] for the number of kink-based entanglements (a) and the scaled number of kink-based entanglements (b) as a function of dimensionless shear rate, Wi_{CR}

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Topic preference: Soft Condensed Matter
Presentation preference (oral/poster): Oral
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Altering Polymer Crystallinity Utilizing Bottlebrush Copolymers

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Abstract: Polymer crystallization has been attracting significant scientific attention as it determines in a large extend the final properties of the materials. Tuning polymer crystallinity emerges as a major challenge and a subject of intense research. On the other hand, polymer brushes are a class of polymers that have attracted considerable research interest because of their properties and their wide range of applications. In this work, we have developed a series of well-defined poly(2 (dimethylamino ethyl methacrylate)-g-poly(ethylene glycol), PDMAEMA-g-PEG bottlebrush copolymers, with different lengths of the side chains aiming to tune PEG crystallinity. The main PDMAEMA chain has a molecular weight of M_n = 44000 g/mol and the graft copolymers were synthesized by chemically attaching methyl terminated PEG chains of different molecular weights (M_n = 500 - 5000 g/mol) by a quaternization reaction on the ternary amine group of PDMAEMA. Graft copolymers comprising single- and mixed-length PEG chains of different mole ratios were synthesized.

The crystallization behavior of all polymers was studied using non-isothermal and isothermal Differential Scanning Calorimetry (DSC) and Small- and Wide-Angle X-ray Scattering (SAXS-WAXS) measurements. Grafting of single PEG chains on the PDMAEMA backbone resulted in a reduced crystallinity compared to the bulk PEG; the crystallinity was reduced even further in the case of mixed-length grafted chains. In this case, the overall crystallinity and the activation energy of the crystallization process decreased with increasing the fraction of PEG chains with lower molecular weight.

Acknowledgements: This research has been partially financed by the EU Horizon Europe Programme (project STOP [Grant Agreement 101057961].

Topic preference: Soft Condensed Matter
Presentation preference (oral/poster): Oral
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Diffusive Filaments in Soft Matter Systems: Modelling Active Colloids and Degrading Microplastic Fibres

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Abstract: Chemically active filaments are ubiquitous in soft condensed matter systems, spanning synthetic microswimmers to degrading microplastic fibres. Their behaviour emerges from complex couplings between surface chemical activity, solute diffusion, and fluid-structure interactions. This work presents a mathematical framework for modelling such diffusive filaments, chemically active bodies that exchange solutes with their environment via surface fluxes.

Central to this approach is Slender Phoretic Theory (SPT), a reduced-order model asymptotically derived to describe solute transport around thin, flexible filaments. By exploiting filament slenderness, SPT transforms the three-dimensional Laplace problem into a one-dimensional integral along the filament's centerline, while accommodating arbitrary geometries, spatially varying activity, and cross-sectional heterogeneity. The theory has been rigorously validated against full numerical simulations using Boundary Element Methods with regularised singularities.

Building on this foundation, we are currently exploring two key applications of SPT within soft matter contexts: (i) autophoretic colloidal filaments and synthetic microbots, and (ii) degrading microplastic fibres in fluid environments. In both cases, SPT provides insight into how local solute fluxes drive filament motion, deformation, or release dynamics, offering predictive power in the design of active matter systems and in understanding pollutant transport at the microscale.

These ongoing investigations demonstrate how a unified theoretical framework can bridge active and passive filamentous soft materials, contributing to a deeper understanding of chemically mediated dynamics in complex, microscale environments.

Topic preference: Soft Condensed Matter
Presentation preference (oral/poster): Oral
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Hierarchical Multi-scale Simulations of Polymers via Atomistic and Chemical-specific Bead Spring Models

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Abstract: The simulations of polymeric systems is a challenging task due to the broad spectrum of time and length scales characterizing them. Atomistic molecular dynamics (MD) simulations provide a detailed investigation of polymers at the atomic scale. To address phenomena at larger length scales, typical bead spring are used. Such models offer a coarser, and computationally more efficient representation of macromolecular chains, allowing for the examination of greater spatial and temporal ranges. In these ranges phenomena like entanglements become emergent, which govern the macroscopic properties of polymeric materials.

Here we provide a systematic hierarchical approach based on a "bottom up" coupling of atomistic and bead spring models. First atomistic MD simulations of relatively short chains (on the order of 100mer) of specific polymeric systems are applied. Then, results of the atomistic simulations are used to parameterized generic bead spring models in order to be applicable for the same polymer systems (chemistries).

The proposed scheme is applied to various unentangled and moderately entangled melts polymer melts, such as poly(ethylene oxide), polystyrene and polyethylene. We compare in detail the structural and dynamical properties of the atomistic and coarse-grained (bead spring) models, providing a detailed spatial and temporal mapping of the bead spring models in order to account for a chemical specificity derived from the atomistic scale. Then, we present results from the atomistic and bead spring MD simulations concerning the thermodynamics (density), structure (pair distribution functions), dynamics (diffusion coefficient) of polymeric systems.

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Topic preference: Soft Condensed Matter
Presentation preference (oral/poster): oral
Full name of presenting author: Artem Tomilo
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Atomic Cluster Expansion Methods for Machine Learning Potentials of Organic Systems

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Abstract: The ab initio computation of energetic and material properties via density functional theory (DFT) constitutes a pivotal advancement in solid-state physics and quantum chemistry [1]**.** However, for soft condensed systems, such as polymers, gels or liquid crystals with a large number of degrees of freedom and no long-range order, the direct application of DFT is still major challenge due to the high computational complexity, and the semi-empirical potentials have a large inaccuracy that is caused by the roughness of the approximation [2]. In this work, we propose a systematic hierarchical approach to derive accurate classical models (force fields) of organic and inorganic systems, using data from DFT calculations, based on atomic cluster expansion formalism. The atomic cluster expansion (ACE) approach is a contemporary method that is a reasonable compromise between the foregoing methods, where on the one hand similar orthonormalised basis functions are used for approximation as in DFT, but on the other hand the sum of the final energy is reduced to obtain the computational complexity as in semi-empirical potentials [3]. Here, we perform a detailed investigation of the application of the ACE approach comparing at the same time, with respect accuracy and computational efficiency, against detailed ab-initio simulations and classical models using semi-empirical potentials. The derivation of the new ACE – based atomistic models is implemented via the state-of-the-art Julia programming language, which ensures fast development due to the ease of learning and high performance of the JIT compiler, which efficiently translates the code into direct machine code instructions at runtime [4]. The proposed approach is applied on the exemplary database MD17 of small organic molecules (aspirin, benzene, ethylene, etc.) for comparing energy calculations and force fields [5].

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WEDNESDAY 17 SEPTEMBER 2025

TALKS – SESSION 3

Topic preference: Magnetism and Strongly Correlated Systems
Presentation preference (oral/poster): Invited Talk
Full name of presenting author: Theodosis Trypiniotis
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Towards purely organic spintronic functionality

Theodossis Trypiniotis

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Abstract: Harnessing the spin degree of freedom has long been a central motivation in spintronics research, both for the advancement of future electronic technologies and, more recently, as a potential route toward quantum computation hardware.In this talk, I will first provide a brief overview of the experimental techniques we employ to study spin-dependent phenomena in organic semiconductor systems, followed by a summary of recent findings, such as, the relationship of the spin orbit strength in organic semiconductors to their molecular conformation. The core of the presentation will highlight our efforts to demonstrate spintronic functionalities in purely organic devices. We have developed highly stable organic radical films, which we use for fabricating radical/ferromagnet bilayer spintronic devices. We have subsequently used these systems to successfully detect spin current emission at room temperature, driven by spin pumping from the organic radical layer alone. Notably, this emission can be reversibly suppressed when the ferromagnetic film is tuned into simultaneous resonance with the radical creating a counter-propagating ‘opposite ’spin current. These results provide an experimental demonstration of a metal-free organic radical layer operating as a source of spin current, opening a new avenue for the development of purely organic spintronic devices.

Topic preference: Low Dimensional Materials
Presentation preference (oral/poster): Oral
Full name of presenting author: Emmanuel Koukaras
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Superlubricity of two-dimensional heterostructures: Insights into Design and Challenges

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Abstract: Superlubricity in two-dimensional (2D) materials offer prospects for ultra-low-friction interfaces in nanoscale systems. We develop tailored interlayer potential (ILP) force fields that have been rigorously benchmarked against high-accuracy periodic density functional theory (DFT) calculations, to probe tribological behavior in heterostructures comprised of combinations of graphene, *h*BN and MoS_2. These ILPs capture registry-dependent adhesion and van der Waals interactions critical for frictional response.

Initial molecular dynamics simulations, compared with existing ILPs, reveal variations in sliding behavior and energy dissipation governed by geometric corrugation. We demonstrate that the choice of DFT supercell size markedly influences optimal ILP parameters and contrast energy-only fits with variants enforcing force (derivative) consistency. Ongoing work extends these benchmarks across diverse twist angles and sliding regimes to assess the emergence and stability of superlubric states.

By identifying model sensitivities and key parameters governing interlayer friction, this work offers insights and foundations for predictive design strategies of tribological phenomena in van der Waals heterostructures and suggests pathways for methodological refinement.

Acknowledgments: The research project is implemented in the framework of H.F.R.I call “Basic Research Financing (Horizontal support of all Sciences)” under the National Recovery and Resilience Plan “Greece 2.0” funded by the European Union – NextGenerationEU (H.F.R.I. Project Number: 15932). Results presented in this work have been produced using the Aristotle University of Thessaloniki (AUTh) High Performance Computing Infrastructure and Resources.

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MONDAY 15 SEPTEMBER 2025

POSTER SESSION A

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Poster
Full name of presenting author: Antria Filippou
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Agar-based breast tissue tumour model phantom for FUS breast applications

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Abstract: In this study, an agar-based phantom which includes a tumour, capable of mimicking cancerous human breast tissue, was developed for focused ultrasound (FUS) applications. The phantom consists of a breast fat tissue mimicking material containing 4% w/v agar and 43 % v/v 2-propanol, developed with an anthropomorphic breast shape. The embedded tumour model was developed in a spherical form using 6% w/v agar and 4% w/v silica. A series of experiments were performed to determine the acoustic, thermal, magnetic and mechanical properties of the fabricated phantom. Acoustic attenuation and ultrasonic propagation speed were measured utilising standard through-transmission and pulse-echo techniques. Thermal properties were determined utilising the transient method, whereas identation tests were performed to estimate the mechanical properties. A clinical 3T MRI scanner was employed to evaluate the T1 and T2 relaxation times. The measured acoustic attenuation coefficients for the breast fat tissue and tumour models were 0.69±0.08 dB/cm·MHz and 1.04±0.03 dB/cm·MHz, respectively, while the corresponding ultrasonic propagation speeds were 1590.7±0.05 m/s and 1532.3±0.2 m/s. For the two compartments, the thermal conductivity was between 0.36-0.55 W/m.K, whereas specific heat capacity ranged between 1798-1853J/kg.K. Regarding mechanical properties, Young's moduli of 416 kPa and 540 kPa were obtained for the breast fat tissue and tumour models, respectively, with the measured T1 and T2 relaxation times being 705.6±27 ms and 125.9 ± 16.2 ms for the breast fat tissue mimic, and 1318.7±77.9 ms and 23.1 ± 2.5 ms for the tumour model. The majority of the measured properties of both phantom components align with corresponding literature-reported values for human breast fat tissue and tumours. Findings indicate that this phantom adequately replicates critical acoustic, thermal, magnetic, and mechanical characteristics of human breast fat tissue and tumours, making it a cost-effective preclinical evaluation.

Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Poster
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Aptamer-functionalized nanoparticles for small molecule detection using SERS

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Abstract: Small molecules play an important role in the pathogenesis and progression of many physiological and pathological processes, especially at early stages. Examples of impactful small molecules include pesticides, drugs, cellular biomarkers and cancer-causing compounds such as acrylamide [1]. Acrylamide, a well-known carcinogen, is commonly found in heated carbohydrate-rich foods such as biscuits, crisps and fries, and given its carcinogenicity, the WHO has set a daily limit on its consumption (0.3–0.8 μg kg^{-1}). The gold-standard in small molecule detection, including acrylamide, involves analytical techniques such as mass spectrometry and chromatography, which have a long turnaround time and can be costly and laborious, limiting their real-life applications [1,2]

Surface-enhanced Raman spectroscopy (SERS), which is an enhanced version of Raman spectroscopy, employing nanoparticles, enables plasmonic signal amplification and the rapid detection and identification of molecules in trace amounts [3,5]. In recent years, one of the most widely used signal amplification strategies in SERS includes the use of aptamers, nucleic acids specific to the molecule of interest. This integrated approach combines the specificity of aptamers with the high sensitivity of SERS, increasing the method's application in real-life applications [3].

SERS substrates are critical in attaining signal enhancement, especially in the case of small molecules such as acrylamide. Gold and silver nanoparticles with various morphologies, multifunctional substrates with multiple functional groups, semiconductors and labelled Raman substrates are widely used [1,2]. An advantage of aptamers includes their ease of modification with dyes, tags or secondary complementary sequences, further enhancing their detection capabilities when combined with SERS [1,2]. As there is growing interest in the advances of nanomaterials in SERS applications, this poster will present the latest advances in the field and the potential for future applications, as well as our preliminary results.

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Topic preference: Advanced Functional Materials
Presentation preference (oral/poster): Poster
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Optical sensing of picric acid based on 2D metal-organic framework nanoleaf embedded with carbon quantum dots

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Abstract: A novel preparation of 2D metal–organic framework (ZIF-8) nanoleaf (ZIF-L) embedded with nitrogen-doped carbon quantum dots (NCQDs) has been successfully developed. NCQDs, produced via hydrothermal treatment of citric acid and ethylenediamine, exhibit an excitation wavelength independence (λ_{ex}-independence) with average diameter 6 nm and a high quantum yield of 84%. Incorporation of NCQDs into ZIF-L framework generates a continuous 2D framework of NCQDs@ZIF-L nanocomposite. Comprehensive characterization was carried out using FTIR, XRD, TEM, and N_2 adsorption–desorption mechanism. The XRD data reveals no significant change in the crystallinity of ZIF-L upon the encapsulation of NCQDs. Notably, the synergetic cooperation between ZIF-L and NCQDs enhances the fluorescence emission due to the availability of free active sites leading to higher adsorption capacity, thereby improving its performance in sensing applications. The NCQDs@ZIF-L nanocomposite synergistically combines active-rich-electron nanospaces with a high surface area, which significantly improves its ability to selectively detect picric acid (PA), a nitroaromatic explosive. The enhanced detection is attributed to the strong hydrogen bonding interactions with the hydroxyl groups of PA. The nanocomposite exhibits excellent fluorescence-based sensing capabilities in aqueous media for PA, achieving a low limit of detection (LOD) of 0.139 µM. Furthermore, the nanocomposite was utilized in real water samples (tap water) spiked with different concentrations of PA. The results showed a high recovery rate (*R %*) reaching 91–102 % and a relative standard deviation (*RSD %*) less than 5 %, showing a promising fluorescent probe for sensitive detection of nitroaromatic compounds under circumstances.

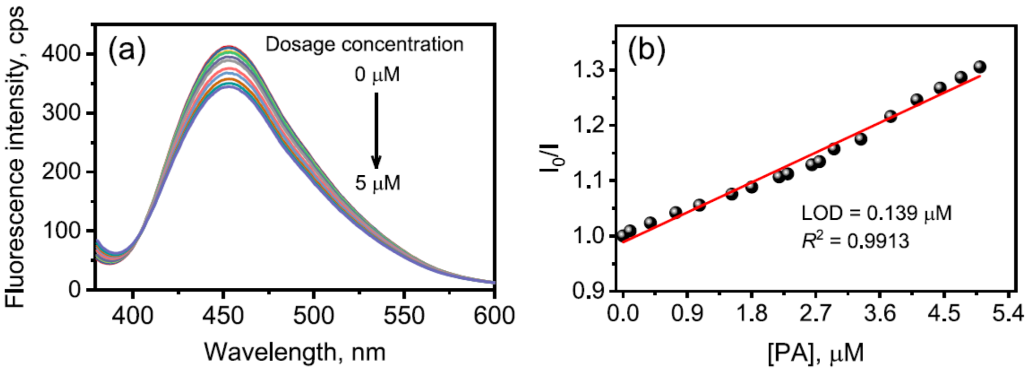

Fig. 1(a) [PA]-fluorescence dependence of NCQDs@ZIF-L nanocomposite in the range 0-5 µM. (b) Stern-Volmer linear plot of NCQDs@ZIF-L nanocomposite.

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Presentation preference (oral/poster): Poster
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Optical spectroscopic study of the $K_2[Ru(bipy)(CN)_4]\cdot3H_2O$ coordination polymer under high pressure

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Abstract: Coordination polymers are hybrid crystalline materials, in which organic ligands connect to metal ions or clusters to produce extended coordination networks, with varied structures and strong luminescence signal. Among them, $K_2[Ru(bipy)(CN)_4]\cdot3H_2O$ (bipy: bipyridine) features the $[Ru(bipy)(CN)_4]^{2-}$ anion, which is strongly solvatochromic, with its absorption and emission spectra being tunable over a wide range in different solvents. In this work, the pressure response of the crystal (triclinic *P*-1 space group, Z=2) is studied by Raman and photoluminescence spectroscopy using a diamond anvil cell for pressure generation and Daphne 7676 oil as pressure transmitting medium.

The Raman spectrum of the studied system can be divided into different spectral regions, depending on the moieties involved in the vibrational modes. Regarding the strong luminescence signal in the 1.5-2.5 eV region, it is composed of different components that originate from the transitions between the ^{3}MLCT (Metal-to-Ligand Charge Transfer) excited state and the vibrational levels of the ground state. Upon pressure increase, most of the Raman peaks shift to higher frequencies due to the bond hardening upon volume contraction. In the pressure range 1.2-2.0 GPa, new Raman peaks appear in the spectrum, distinguished from the initial peaks because of the different pressure slopes of their frequencies. Moreover, above 4.5 GPa additional and more significant changes occur with respect to the number of the Raman peaks, their frequencies and pressure coefficients, as well their relative intensities. The observed changes suggest the occurrence of pressure-induced structural transitions, which are fully reversible upon pressure release. These transitions are less pronounced in the photoluminescence spectrum, with changes being more evident in its high energy side.

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A novel, water stable Zn-MOF as a photoluminescent sensor and sorbent for selected pharmaceutical compounds

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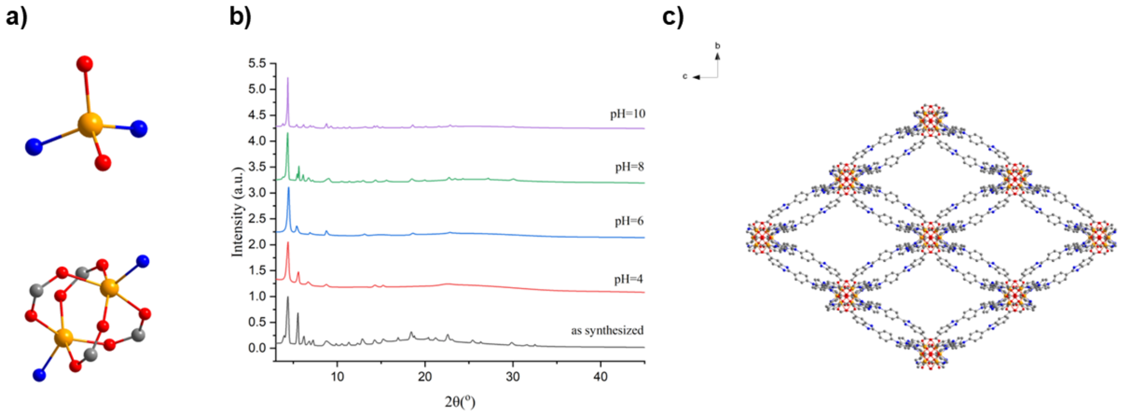
Abstract: Metal – Organic Frameworks (MOFs) are an emerging class of functional materials, due to their unique characteristics and properties. Their porous nature, large surface area, tuneable pore size and diverse functionality render MOFs highly suitable for different possible applications. Luminescent MOFs, also known as LMOFs, are isolated by the combination of suitable ligands and metal ions during synthesis. LMOFs have been proved to be very promising candidate materials for detection of various hazardous, illicit or biologically important species. In this work, we report the synthesis and characterization of a novel three-dimensional, zinc-based MOF, named ZnTBIA. Interestingly, the compound ZnTBIA is a rare example of Zn-MOFs that retains its crystallinity when immersed in aqueous solutions and additionally exhibits ligand-based photoluminescence. These properties enabled us to evaluate its ability to detect and adsorb pharmaceuticals in aqueous solutions. Our studies focused in the detection and the removal of three positively charged pharmaceuticals, with antipsychotic action. Our findings indicate that ZnTBIA can efficiently detect all three pharmaceuticals with LOD values comparable to their concentrations in real-life wastewater. Additionally, ZnTBIA is an efficient adsorbent, presenting high qmax values in the adsorption experiments for each pharmaceutical. These findings emphasize the broad applicability and potential of Metal-Organic Frameworks in both analytical and environmental fields.



a) Zn^{2+} forms tetrahedral geometry and paddle-wheel b) pXRD diagrams when immersed in aqueous solutions of pH 4 to 10 c) three-dimensional representation across a-axis of the discussed MOF

Topic preference: Advanced Functional Materials
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Spatially Controlled Hydrothermal Synthesis of CuO Nanoparticles on Silicon Wafer Using Optical Lithography

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Abstract: Nanostructured transition metal oxides (MOs) represent a critical class of nanomaterials essential for the development of innovative functional and smart materials, with widespread applications in electronics, photonics, and environmental technologies. Among these, cupric oxide (CuO) nanostructures—recognized as p-type semiconductors with narrow band gaps and low-cost synthesis routes—have attracted significant attention for their potential in nanoscale electronic, optoelectronic, and sensing devices. A key challenge in realizing these applications lies in achieving precise spatial control over the placement of nanomaterials, which is crucial for the advancement of microelectronic and sensor systems. In this context, lithographic techniques remain the primary approach for enabling well-defined organization of nanostructures.

This study focuses on identifying an optimal method for synthesizing CuO nanoparticles on selectively patterned regions of silicon substrates, targeting their application in gas sensor technologies. A two-step hydrothermal process, combined with an optimized sol-gel seeding approach, was employed to ensure high crystallinity of the CuO nanostructures. The silicon surfaces were meticulously prepared through piranha solution treatment, sequential acetone–propanol cleaning, and a final ozone-UV activation. The sol-gel precursor was then deposited onto the substrate, followed by optical lithography (using either positive or negative tone resists) to define the desired pattern. Hydrothermal growth was subsequently performed to synthesize CuO nanostructures selectively within the lithographically defined areas.

The resulting CuO nanoparticles were systematically characterized using optical microscopy, scanning electron microscopy (SEM), and X-ray diffraction (XRD) to evaluate their morphology, crystallinity, and compositional uniformity. The results validate the efficacy of combining optical lithography with hydrothermal synthesis as a scalable and reliable approach for fabricating organized arrays of CuO nanostructures. This method provides a promising route for the integration of transition metal oxide nanomaterials into next-generation functional device architectures, particularly for gas sensing applications.

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Topic preference: Advanced Functional Materials
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Hydrothermal Synthesis of Inorganic Materials

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Abstract: This work focuses on the study and development of inorganic materials based on the binary silicon-oxygen (Si-O) and/or zirconium-oxygen (Zr-O) binary systems. The main objective is the isolation of inorganic materials with improved structural and morphological properties, using wet chemistry techniques. For the synthesis of these materials, Si- and Zr- precursor compounds such as tetraethyl orthosilicate (TEOS) or zirconium oxychloride ($ZrOCl_2$) were used in addition to various organic surfactants such as cetyltrimethylammonium bromide (CTAB), sodium dodecyl sulfate (SDS) and polyethylene glycol 4000 (PEG4000). In addition, aqueous solutions of NaOH and/or NH_4OH were used to adjust the pH and enhance the hydrolysis and condensation processes. The significance of this research lies in the ability to produce nanostructured materials with controlled characteristics, such as porous structure and crystallinity. All isolated materials were characterized using FT-IR spectroscopy, XRD and SEM for chemical bonding, crystallinity, and morphology, respectively. The comparative study of the surfactant type and pH agent shows that these two parameters have a considerable impact on the final structure and properties of the Si-O and Zr-O based materials. This work demonstrates a contribution to designing tailored inorganic nanomaterials for catalysis, energy storage and biomedical applications.

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Experimental investigation of the tensile and shear properties of steel foam hollow sphere assemblies

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Abstract Metal foams are artificial materials that replicate structures of nature, such as bones or wood, etc., that exhibit interesting physical and mechanical properties with a wide range of applications in the industry (Zhao *et al.*, 2017; Patel *et al.*, 2018). The mechanical properties under compression are probably the most well-studied for metal foams and porous metals, as indicated by the publication of a standard method for the compression of porous metals (ISO 13314, 2011), the only dedicated standard for metal foams and porous metals. Though compressive performance and corresponding energy absorption characteristics can be satisfied with the aforementioned standard, the lack of standards or other reliable protocols for determining mechanical properties in tension and shear, despite different efforts (Kalpakoglou and Yiatros, 2022) is a barrier for further industrial application of such materials. We will present the specimen prototyping steps and the experimental procedure to test and determine mechanical properties such as Young's Elastic Modulus, Shear Modulus, maximum tensile and shear strength. The outcome is a proposed methodology for studying similar assemblies under tensile and shear loading and an attempt to explain the differences between past theoretical and experimental results. For this investigation, we used metal foam hollow spheres of two different diameters (2 mm and 4 mm) for the specimens in question.

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Presentation preference (oral/poster): Poster
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Microstructural features, physico-mechanical properties, and wear behavior of dental translucent polychromic multilayer zirconia of hybrid composition prepared by milling technology

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Abstract: The present study aims in characterizing the microstructure, mechanical properties, and wear behaviour of the enamel, transition, and dentine layers, which comprise the polychromic multilayer zirconia materials of hybrid composition fabricated by digital milling. Prismatic blocks were fabricated from commercial pre-sintered dental polychromic multilayer zirconia of hybrid composition, IPS e.max ZirCAD Prime (medium and high translucency, from the dentine to the incisal layer) and 3D Pro ML (translucency gradient, from the dentine to the incisal layer) by milling technique, and subsequently cut into three distinct parts to separate the enamel, transition, and dentine layers. The samples were sintered, thermally treated (similarly to the glazing procedure), and polished for characterization. Their microstructures (through SEM and XRD), mechanical properties (through nanoindentation and microhardness), and wear behaviours (through scratch test), were investigated. The resultant materials had a homogeneous, dense, and well crystallized nanostructure comprising tetragonal and cubic zirconia. The grain size decreased from the enamel to dentine layer and a similar trend was observed for the mechanical properties. Nevertheless, the three layers demonstrated similar dynamic friction coefficient (μ_d). The differences in the abovementioned properties of the three layers had a minor influence on the wear behavior of the entire multilayer zirconia material. Dental restorations produced from polychromic multilayer zirconia of hybrid composition by milling technology are strong, non-fragile, and esthetic materials, anticipating good performance in oral cavity.

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Self-Healing Solid Polymer Electrolytes Based on Nanostructured Polymer Particles for Solid-Sate Batteries

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Abstract: Soft materials such as polymers are prone to structural damage caused by mechanical loads or environmental factors, leading to embrittlement, cracking, and functional degradation. This compromises the lifetime and reliability of polymer-based technologies while increasing their economic and environmental costs. To address this, significant research has focused on developing self-healing polymer materials capable of recovering performance after minor structural damage. However, achieving intrinsic self-healing in stiff, mechanically robust materials remains a major challenge due to the inherent trade-off between mechanical strength and dynamic healing capability. Strong interactions enhance toughness but restrict molecular mobility, limiting self-healing, whereas weak interactions enable healing but reduce mechanical integrity.

In this work, we present a novel macromolecular strategy to overcome this dilemma by designing hard–soft multiphase nanostructured polymer materials based on high-functionality mikto-arm star copolymers. Owing to their tailored molecular architecture and colloid-like structure, these materials self-assemble into patchy, hard–soft nanostructured particles, combining mechanical robustness with dynamic healing.

The resulting materials exhibit solid-like behavior with high storage moduli ($G' \gg G''$, $G' \approx 10$ MPa) alongside rapid and autonomous self-healing after mechanical deformation. Remarkably, under nonlinear shear, the materials yield and flow, followed by complete structural recovery upon flow cessation, making them not only tough and self-healing but also processable and extrudable, broadening their application potential in sustainable, high-performance polymer technologies.

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Dissecting the role of molecular structure and film microstructure in photophysical processes in ternary blends of organic polymeric semiconductors with non-fullerene acceptors

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Abstract: Improving the performance of organic solar cells (OSCs) relies on refining both the molecular design and film microstructure to achieve efficient charge generation and suppress recombination losses [1],[2],[3]. However, the complex interplay between molecular structure, microstructure, and excited state dynamics in multi-component blends remains a critical challenge. Optimizing the photophysical landscape of organic solar cell blends requires a thorough understanding of how the molecular structure and film microstructure regulate the excited state dynamics. Here, we investigate blends of the PTB7-Th (PCE10) polymer donor with two non-fullerene acceptors (NFAs) differing in side chain architecture (O/EH-IDTBR), using ultrafast Transient Absorption Spectroscopy (TAS) to investigate the effect of molecular structure, addition of the third component (O-IDFBR), and thermal annealing on the charge generation and recombination pathways. We complement the photophysical insights with structural information from the molecular scale to microstructure and morphology using Resonance Raman (RR) spectroscopy, Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS) and Atomic Force Microscopy (AFM). RR provided insight into the effects of blending, NFA side-chain substitution, and thermal annealing on molecular conformation, while GIWAXS and AFM revealed changes in crystallinity, molecular packing and surface morphology evolution under the same conditions. We find that blending leads to loss of crystallinity of all the components in the films, which is, however, recovered with thermal annealing, but only for the polymer, leading to phase separation. Importantly, we show that the combination of side-chain engineering and thermal annealing - rather than blending alone - modulates the formation and dynamics of photoexcited species, as revealed by TAS.

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Optical probes for in-situ monitoring of charge recombination in organic photovoltaic devices

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Abstract: Over the last decade, the power conversion efficiencies (PCEs) of organic photovoltaic (OPV) devices have advanced significantly owing to the introduction of a new class of acceptor materials, the so-called non-fullerene acceptors (NFAs) boosting PCEs to 20% [1]. However, OPV devices are far from competing with inorganic solar cells mainly because of loss channels due to charge recombination. Following photon absorption by the nanostructured OPV composite, the formed excitons undergo charge transfer (CT) reactions at NFA/donor interfaces, thereby creating partially separated electron-hole pairs. Owing to the appropriate microstructure of the OPV blend, free carriers are formed that transport towards the device electrodes, where they can be extracted contributing to photocurrent generation. However, device performance degrades when free carriers recombine non-geminately prior to extraction. Advantageously, non-geminate charge recombination may re-activate the CT state of the OPV blend hence offering a unique probe to monitor these losses. In this work, we propose a novel spectroscopic methodology to quantify charge recombination losses in operative OPV devices [2,3]. Time-gated photoluminescence (PL) spectroscopy is an ideal probing tool to monitor the activation of the PL spectral signature CT states at variable delays after photoexcitation. The time-dependent PL intensity of CT states, as monitored at different photoexcitation power densities, serves as a proxy of the non-geminate charge recombination losses. Hereby, we benchmark a well-studied system, PS:PDI, with a modern NFA-based OPV blend, in order to quantify the difference in recombination dynamics by conducting detailed time-gated PL spectroscopic studies (in the ns-ms time range) to validate our proposed methodology.

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Topic preference: Photonics and Optoelectronics
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Molecular Interactions and Structural Stabilization in Hybrid Interfaces for Optoelectronic Applications: A Multiscale Approach

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Abstract: Integrating the phosphorescent organometallic complexes with the conducting polymer to make a hybrid composite is a promising way to improve the performance of the optoelectronic and sensing devices. Our investigation employs the multiscale simulations and focuses on the molecular interactions and the structural arrangement of metal-centered π-conjugated complex (PtOEP) with different substrates: the sulfonated polymer blend (PEDOT: PSS) and the metal oxides (ZnO) surface. At first, quantum chemical methods were used to optimize the complex and correctly capture the coordination geometries and the electronic environment. Then, the classical molecular dynamics simulations were employed to predict the behaviour of the polymer matrix in the solvated condition. Extensive atomistic models of hybrid interfaces reaching sizes of up to 10 nm are being created to replicate realistic device-like environments, and extended molecular dynamics simulations (100-200 ns) will be employed to elucidate the structural evolution, dynamic behaviour, and substrate-induced confinement effects. Guided by these atomistic insights, we will further investigate how interfacial morphology and local electronic environments influence critical electro-optical phenomena, including exciton confinement, non-radiative decay, and charge transport at the substrate complex interface. This investigation attempts to provide a thorough molecular-level understanding of how substrate selection affects hybrid interface structure and function by combining multiscale computational modelling with experimental electro-optical characterisation. The results will establish a basis for the systematic design of hybrid materials with adjustable optoelectronic characteristics, tailored for optoelectronic and sensing applications.

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Triplet–triplet annihilation induced photon energy up-conversion as a pathway to mitigate transmission losses in excitonic platforms

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Abstract: Triplet-triplet annihilation-induced photon energy up-conversion (TTA-UC) refers to a photochemical process occurring in composite systems of small organic molecular and π-conjugated polymeric emitters whereby delayed luminescence is produced with photon energies higher than the photon energy used for photoexciting the composite. TTA-UC is particularly attractive as a wavelength-shifting tool to enable photoactuation *i.e.* the sensitization of organic solar cells at long wavelengths of incoming light where the photoactive layer of the OSC device is transparent. Encouraging results have been presented recently on the quantum yield (Φ) of the archetypical TTA-UC system of the 9,10 di-phenyl anthracene (DPA) emitter mixed with the (2,3,7,8,12,13,17,18-octaethyl-porphyrinato) platinum^{II} (PtOEP) metallorganic sensitizer [1]; a green-to-blue Φ_{TTA-UC} as high as 8% was reported for solution-processable solid-state DPA:PtOEP films [2]. Nevertheless, the binary nature of the DPA:PtOEP composite film introduces severe implications in terms of device engineering aspects, and the incorporation of the DPA:PtOEP up-converting interlayers in OSC devices with vertically-stacked geometries is hard to achieve [3]. Herein, we present an alternative TTA-UC excited state pathway that promises to establish a feasible route towards TTA-UC sensitized photoactive devices of vertically-configured geometry. In particular, we focus on the spectroscopic study of the TTA-UC system comprising the DPA emitter mixed with the (3,3,7,8,12,13,17,18-octaethylporphyrin-22,24-diid-2-one) platinum^{II} (PtOEP-K) metallorganic complex. [3]. Although the TET process from PtOEP-K to DPA is energetically improbable, a green-to-blue Φ_{TTA-UC}= 2.5 % is obtained with an excitation fluence of 1.1 × 10^{20} cm^{-2} s^{-1} (4 W/cm^2) of 532 nm CW-laser excitation [3]. Time-gated photoluminescence spectroscopic experiments (in the ns – ms time range) are conducted for PtOEP-K-only and DPA:PtOEP-K degassed solutions in toluene to unravel the operational mechanism of this intriguing photophysical phenomenon.

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Room-Temperature Nanosecond Amplified Spontaneous Emission from Tin Iodide Perovskite Nanostructures

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Abstract: Lead halide perovskite nanocrystals (NCs) exhibit remarkable stimulated emission properties, facilitating efficient optically pumped lasing across the visible spectrum. While their tin-based counterparts don't match such achievements yet, they offer the prospect of a greener, lead-free alternative, also extending access to the important near-infrared region. In this work, recent advancements in the synthesis of colloidal $CsSnI_3$ nanostructures are employed to demonstrate that films of these nanomaterials are capable of sustaining amplified spontaneous emission (ASE) under nanosecond pulsed optical excitation at cryogenic temperatures up to 150 K. Further optimization is achieved by incorporating multilayered structures of $CsSnI_3$ NCs and cellulose acetate (CA), which not only provide improved optical waveguiding within the higher-index $CsSnI_3$ NC layer but also enable the assembly of the active region through uniform thin alternating layers rather than a single thick, disordered NC slab. Using this approach, nanosecond, room-temperature ASE with a threshold of ~870 $\mu J/cm^2$ and a net modal gain of ~25 cm^{-1} is demonstrated. This work not only challenges the perceived limitations of unstable lead-free perovskite NCs but also outlines a viable strategy for their integration into practical, nanosecond-pumped photonic devices.

TUESDAY 16 SEPTEMBER 2025

POSTER SESSION B

Topic preference: Low Dimensional Materials
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Optimizing the Optoelectronic Properties in InAs Colloidal Quantum Dot Thin Films via Post-Deposition Processing

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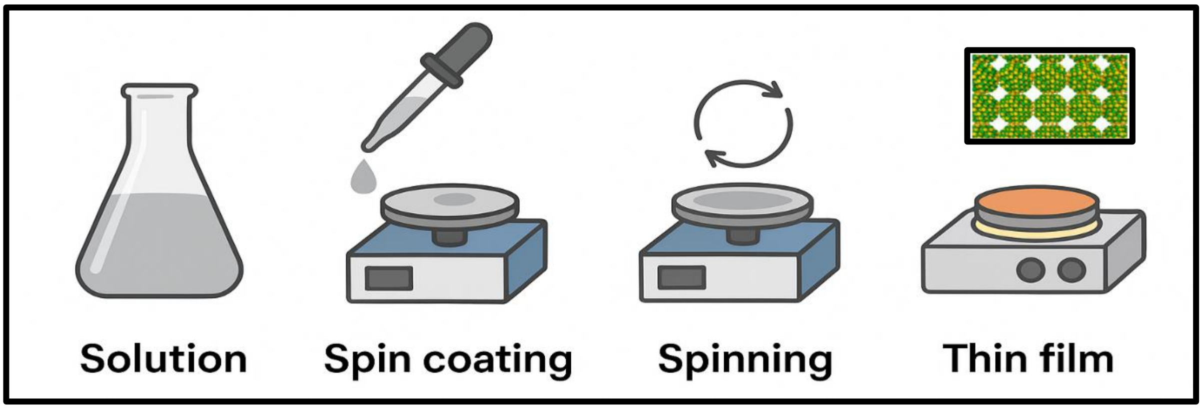
Abstract: InAs colloidal quantum dots (CQDs) have recently gained attention as promising low-toxicity alternatives to the more established lead- and mercury-based infrared CQDs. Realizing the full potential of InAs CQDs in solid-state optoelectronic devices requires advances in film deposition and processability, effective surface trap passivation, and enhanced inter-dot electronic transport. In this work, we investigate the impact of post-synthetic treatments based on the ionic liquid salt, 1-ethyl-3-methylimidazolium iodide (EMII), on the optoelectronic properties of InAs CQD films using optical spectroscopy and electro-optical techniques. Upon optimization, EMII treatment is found to improve the film morphology, surface chemistry, photoluminescence, and inter-dot electronic coupling within the CQD films. These findings provide new insight into the role of ionic salt treatment and ligands in CQD surface engineering and offer a versatile strategy for optimizing InAs thin film materials for optoelectronic applications.



Topic preference: Low Dimensional Materials
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Optical Properties of Thin Films of Tin Iodide Perovskite Nanostructures

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Abstract: Tin-based perovskite nanocrystals (NCs) are a more environmentally friendly alternative to lead-based counterparts, but they are still hampered by tin oxidation and structural polymorphism. These stability issues worsen in the solid state due to greater exposure to moisture and oxygen, which restricts the number of available thin-film studies on tin halide nanostructures. In this work, we present a spectroscopic investigation of 3D $CsSnI_3$ NCs coexisting with a minor fraction of 2D Ruddlesden-Popper nanosheets (NSs). Encapsulating the nanocrystals in a polystyrene matrix yields solids that remain stable under oxygen-free conditions, even after repeated thermal cycling. At room temperature, pump–probe and photoluminescence measurements show prominent excitonic features from the 3D NCs and weaker ones from the 2D $(R\text{-}NH_3)_2SnI_4$ NSs, with bleaching and emission lifetimes on the order of 0.1 and 1 ns, respectively. Hyperspectral microscopy and spectroscopic data suggest that exciton behaviour is governed primarily by intrinsic recombination, with minimal effects from NC–NC or NC–NS electronic coupling. However, structural interactions, for instance NS attachment to NC surfaces, may contribute to exciton trapping and bound-exciton emission observed at cryogenic temperatures [1].

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Photophysics of Indium Arsenide Colloidal Quantum Dots

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Abstract: Colloidal quantum dots (QDs) are promising nanomaterials for next-generation photonics due to their unique size-tunable electronic states, solution processability and excellent optical properties. Within the expanding QD family, infrared (IR)-active materials hold promise for applications in telecommunications, bioimaging, photovoltaics, and sensing. Indium arsenide (InAs) QDs emerged recently as promising low-toxicity alternatives to traditional lead- and mercury-based chalcogenide IR QDs. Recent developments in synthetic methodologies have enabled the production of sufficiently stable, crystalline InAs QDs. Despite the progress, many aspects of the fundamental optoelectronic properties of such QDs especially in the form of thin films are still elusive.

This work aims to address some of the gaps in the current understanding of InAs QD solid state photophysics by spectroscopic studies focusing on the interplay of exciton radiative recombination versus exciton trapping and the impact of thin shells on such competition. Towards such goal, temperature dependent, steady-state, and time-resolved photoluminescence (PL) measurements are employed as the main probing tool to investigate exciton energetics and dynamics in thin films of InAs core, and InAs/ZnS, InAs/ZnSe core/shell QD systems. This investigation provides insight into the QD exciton physics and provides estimates of important figures of merit for the QD solids that include exciton–phonon coupling, surface trap depth and thermal escape barriers.

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Presentation preference (oral/poster): Poster
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Graphene Gas (O_2)-Bubbling Electrode as a Dynamic Surface for a Sustainable Electro Wastewater Treatment Plant

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Abstract: Graphene possesses an exceptional combination of properties, of interest to various practical applications in electronic, optoelectronic, and energy storage devices. In this study, a 3D Graphene foam with electrocatalytic activity was prepared for use as oxygen(O_2)-bubbling electrode in a hybrid electrocoagulation treatment reactor to achieve efficient degradation of organic pollutants. The initial operation of the reactor was for treating oily effluent (bilge), which is a high-strength industrial wastewater, produced by every motorized component and includes all the water and wastewater derived from the bilges of a ship. 3D Graphene was synthesised by utilising nickel foam as a catalyst in a thermally-enhanced Chemical Vapour Deposition (T-CVD) process, with methane as the carbon source. Raman spectroscopy is used to evaluate the influence of deposition time on the thickness of graphene layers, as well as to assess its structural properties. Considering the most notable metric for the removal of pollution from bilge wastewater, the Chemical Oxygen Demand (COD) reduction, the Fe-Graphene electrodes reduced the COD pollution by 15% more, compared to the Fe-Fe electrode combination.

Topic preference: Low Dimensional Materials
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Exploring Superlubricity in Graphene–Based Heterostructures through Tailored Interlayer Force Fields

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Abstract: Superlubricity in two-dimensional (2D) materials presents a compelling opportunity for enabling ultra-low-friction interfaces in nanoscale systems. In this study, we develop and evaluate tailored interlayer potential (ILP) force fields to explore the tribological behavior of graphene–MoS_2 and graphene–hBN heterostructures. These ILPs incorporate enhanced representations of lattice mismatch and van der Waals interactions, which are critical for capturing frictional characteristics at the atomic scale.
Initial molecular dynamics simulations and comparative analyses with existing ILP models reveal distinct variations in sliding behavior and interfacial energy dissipation dependent on geometry corrugation. We investigate the sensitivity of the onset and manifestation of superlubricity on the potential energy landscape, using both detailed and simplified atomistic representations. Ongoing simulations aim to extend these findings under varied sliding conditions and geometrical configurations, with particular attention to the emergence and stability of superlubric regimes. By identifying key parameters that govern interlayer friction, this work contributes to a broader understanding of how theoretical modelling influences observed tribological phenomena in van der Waals heterostructures.
These insights offer a foundation for predictive design strategies that leverage atomically engineered interfaces in advanced 2D materials heterostructures.

Acknowledgments: The research project is implemented in the framework of H.F.R.I call “Basic Research Financing (Horizontal support of all Sciences)” under the National Recovery and Resilience Plan “Greece 2.0” funded by the European Union – NextGenerationEU (H.F.R.I. Project Number: 15932). Results presented in this work have been produced using the Aristotle University of Thessaloniki (AUTh) High Performance Computing Infrastructure and Resources.

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Topic preference: Low Dimensional Materials
Presentation preference (oral/poster): Poster
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Self-Energy and Interaction Effects in Graphene from a Quantum Field Theory Approach

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Abstract: We present a quantum field theoretical analysis of Dirac fermions in graphene, focusing on their interactions with electromagnetic fields and the emergence of a mass gap due to symmetry breaking. Starting from an effective Lagrangian model, we compute the one-loop quantum corrections to the fermion propagator by evaluating the two-point Green's function. A mass term is introduced to model the energy gap between the conduction and valence bands, enabling us to explore scenarios where graphene deviates from its gapless, semimetallic behavior. To regularize the theory, we employ Dimensional Regularization, which proves particularly effective in the relativistic limit where the Fermi velocity approaches the speed of light. Our results provide analytic expressions for the fermion self-energy and demonstrate how the Fermi velocity receives momentum-dependent quantum corrections. We also show that in the presence of interactions, a finite energy gap may emerge, with direct implications for graphene-based nanoelectronic applications. This work bridges high-energy theoretical methods with condensed matter phenomena in two-dimensional materials.

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Presentation preference (oral/poster): Poster
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Modeling the response of a one-dimensional magnetic cylinder under an external magnetic field of any form

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Abstract: In this work, we present a comprehensive analytical framework for understanding the static/quasi-static magnetic response of one-dimensional cylindrical magnetic structures (e.g. micro/nano-wires of superconducting low-T_C Nb and ferromagnetic iron oxides Fe_3O_4). Focusing on a linear, homogeneous, and isotropic magnetic cylinder with intrinsic magnetic susceptibility, χ_m^{int}, we explore its response to an arbitrary external magnetic pseudopotential/field, $U_{m,ext}/\mathbf{H}_{ext}$, that does not vary along the z axis, originating from primary sources located outside the magnetic cylinder. The system under consideration is infinitely long along the z-axis. Using an expansion-based method, we derive universal expressions for the induced internal magnetic pseudopotential/field, $U_{m,int}/\mathbf{H}_{int}$, for both the inside and the outside of the cylinder, resulting from the secondary source of bound pseudocharges produced by the external pseudopotential/field, $U_{m,ext}/\mathbf{H}_{ext}$. From these, closed-form solutions, the total magnetic pseudopotential/field, $U_m = U_{m,ext} + U_{m,int}/\mathbf{H} = \mathbf{H}_{ext} + \mathbf{H}_{int}$ and magnetic polarization, $\mathbf{M}$, are obtained. Notably, these results are general and can be applied to any external field configuration without re-solving the problem from the beginning. A key outcome of this study is the identification of mode-independent expressions of both the depolarization factor, N, and the extrinsic magnetic susceptibility, χ_m^{ext}. These universal relations between internal and external fields offer practical tools for the design and analysis of cylindrical magnetic components, particularly in the context of low-dimensional materials.

Topic preference: Magnetism and Strongly Correlated Systems
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Designing High-Spin Organic Materials: The Rylenediimide-Fused Blatter Radicals

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Abstract: The development of organic spintronic materials requires open-shell molecules that are both thermally robust and magnetically active under ambient conditions. In this work, we present rylenediimide (RI)-fused 1,2,4-benzotriazin-4-yls (Blatter radicals) as a promising class of high-spin organic compounds that meet these criteria.

Density functional theory (DFT) calculations demonstrate that fusion of a triazinyl moiety onto the RI core increases molecular rigidity and facilitates extensive spin delocalization across the π-conjugated framework. Notably, this delocalization is retained despite steric interactions that introduce deviations from planarity.

Electronic structure analysis identifies three dominant resonance forms: (1) Kekulé-type (aromatic or quinoidal) structures, (2) zwitterionic biscyanine species, and (3) thermodynamically stabilized diradical conjugates (Scheme 1). The latter exhibit narrow singlet–triplet energy gaps (ΔE_{ST} ranging from –1.3 to 3.8 kcal/mol), indicating facile thermal or optical access to the triplet state. This low-energy interconversion suggests a viable platform for switchable spin states.

Overall, RI-fused Blatter radicals combine chemical stability with tunable electronic and magnetic properties, positioning them as versatile building blocks for the design of advanced organic spintronic materials.

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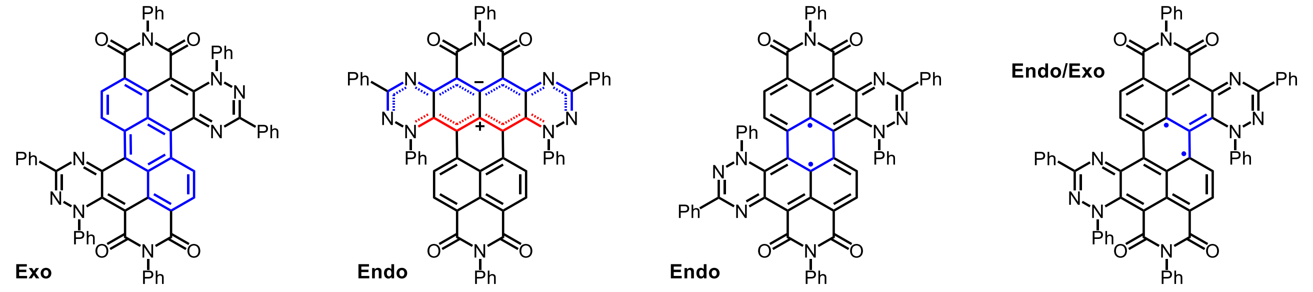

ΔE_{ST} (6-31G) = -7.59 kcal/mol
ΔE_{ST} (6311G+(2d,p) = -8.31 kcal/mol

ΔE_{ST} (6-31G) = -9.57 kcal/mol

ΔE_{ST} (6-31G) = -0.93 kcal/mol
ΔE_{ST} (6311G+(2d,p) = -1.29 kcal/mol

ΔE_{ST} (6-31G) = -2.69 kcal/mol
ΔE_{ST} (6311G+(2d,p) = -3.54 kcal/mol

Scheme 1. Examples of resonance forms of rylenediimide (RI)-fused Blatter radicals.

Topic preference: Magnetism and Strongly Correlated Systems
Presentation preference (oral/poster): Poster
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Unravelling the Spin Dimensionality of a Metal-free Organic Radical Crystal

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Abstract: Materials that exhibit low dimensional spin properties have recently been attracting particular attention with potential applications in emerging technologies such as quantum computing and spintronics.[1,2] However, low dimensional magnetism in metal-free organic materials is very rarely reported possibly due to weak exchange interactions and magnetic anisotropy.[3] Nevertheless, this information is a key element in the effort to identify candidate materials to replace inorganic ferromagnets with metal-free organic equivalents as spin sources.
Here we present an experimental investigation of spin dimensionality of a Blatter radical derivative (BRD) single crystal at room temperature. This was achieved by using Electron Spin Resonance (ESR) technique at an excitation frequency of 9.4 GHz and ESR spectra were recorded in three mutually perpendicular planes aligned with crystal axes which were indicated by the assistance of the X-ray diffraction technique. By analysing the angular dependence of the resonance field and of the linewidth, the signature of two-dimensional magnetic structure was detected, proving that BRD single crystal can be a potential metal-free organic testbed to act as a spin source.

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Topic preference: Magnetism and Strongly Correlated Systems
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Mathematical modeling and experimental realization on poly-crystalline and single-crystalline high-Tc superconductors $YBa_2Cu_3O_{7-\delta}$ and $Bi_{2-x}Pb_xSr_2Ca_2Cu_3O_{10+y}$ via AC magnetic susceptibility: Investigation of the second superconducting transition observed in poly-crystalline samples

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Abstract: AC magnetic susceptibility (ACMS) is a powerful and non-invasive technique for probing the magnetic properties of superconducting materials. In this work, we utilize ACMS to investigate the behaviour of poly-crystalline high-Tc superconductors $YBa_2Cu_3O_{7-\delta}$ and $Bi_{2-x}Pb_xSr_2Ca_2Cu_3O_{10+y}$ and single-crystalline $YBa_2Cu_3O_{7-\delta}$. From the raw measurements, we directly obtain the so-called extrinsic ACMS of each specimen. By accounting for material-specific characteristics (e.g. geometry, demagnetizing effects, etc) we determine the truly intrinsic ACMS of the parent materials. Notably, this is achieved without the need for any calibration specimen. Special focus is placed on the detailed analysis of a second transition observed in both $YBa_2Cu_3O_{7-\delta}$ and $Bi_{2-x}Pb_xSr_2Ca_2Cu_3O_{10+y}$ polycrystalline specimens. By systematically varying the rms value of the externally applied magnetic field, $\mathrm{B}_{\mathrm{ac}}^{\mathrm{rms}}$, over three orders of magnitude at a fixed low frequency, we tracked the evolution of the characteristic temperature, $\mathrm{T}^{*}(\mathrm{B}_{\mathrm{ac}}^{\mathrm{rms}})$, which marks the boundary between linear and non-linear diamagnetic response. A clear, approximately linear dependence of, $\mathrm{T}^{*}(\mathrm{B}_{\mathrm{ac}}^{\mathrm{rms}})$, was recorded, offering valuable insight into the field-induced dynamics of the superconducting state. This study highlights the sensitivity of high-Tc superconductors to small variations in external ac magnetic fields and provides a robust experimental basis for further theoretical modeling of their magnetic response.

Topic preference: Soft Condensed Matter
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Temperature-dependent Resonance Raman spectroscopy of polymeric semiconductors

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Abstract: Temperature-dependent absorption measurements of organic semiconductor thin films universally show a slight red shift with temperature decrease, which is often interpreted as an increase in polymer planarity and conjugation length. However, no structural data from vibrational spectroscopy support this assumption. Here, we employ temperature-dependent Resonance Raman (RR) spectroscopy to understand how temperature affects the chain conformation and thus the photophysical properties of polythiophene derivatives (a) forming either H- or more J-like photophysical aggregates, (b) blended with high dielectric, insulating polymers, or (c) substituted with hydrogen-bonding side chains. In all cases, we find an increase in the polymer backbone torsional disorder when cooling, attested by upshifts in the thiophene C=C symmetric stretch and decrease in the ratio between the ordered and disordered population in the film. Association of the vibrational band upshift with reduced anharmonicity at lower temperatures is discounted from observation of the C=C overtone bands with temperature. Interestingly, we observe a step change in the peak centroid and relative intensity trends with temperature, observed at a temperature that corresponds to the alkyl side-chain relaxation, as revealed from dynamic mechanical thermal analysis. This highlights that the side-chain degrees of freedom are closely coupled to the backbone torsional mobility and can be responsible for modification of excitonic coupling. The results suggest that interpretation of the optical spectra is not as simple as described in the literature so far, but a combination of the structural information obtained by RR and excitonic models for photophysical aggregates are necessary to understand the optical properties.

Topic preference: Soft Condensed Matter
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Effect of CQDs on the nematic order and rotational viscosity of 8CB

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Abstract: We prepared soft nanocomposites of the liquid crystal 8CB doped with Carbon Quantum Dots (CQDs). The homogeneity and microstructure of the samples were examined in situ using fluorescence microscopy and polarized optical microscopy, respectively. We measured the birefringence, phase transition temperatures and Freedericksz-threshold voltage of nematic cells in splay geometry. The influence of CQDs on the orientational order parameter S was investigated as a function of temperature and doping concentration. We also measured the switching times as a function of temperature, applied field amplitude, and sample composition. By combining these results with the existing dynamic theory of nematic liquid crystals, we argue for the contribution of the elastic constants and rotational viscosity γ in the switching times across the nematic range. Of note, we focus on the pretransitional divergence observed upon cooling near the nematic–smectic-A transition. Furthermore, using existing models from the literature, we estimate the activation energy associated with the rotational viscosity, and evaluate the effect of the CQDs on the power-law dependence of γ on S.

Topic preference: Soft Condensed Matter
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High pressure Raman study of crystalline 9,9´-spirobifluorene up to 8 GPa

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Abstract: Polycyclic aromatic hydrocarbons (PAHs) are organic compounds of two or more interconnected aromatic rings with remarkable physical and chemical properties, caused by the delocalization of π-electrons. The formation of spiro compounds, consisting of two mutually perpendicular π-systems, can improve the stability of the low-molecular-weight PAH molecules, which is vital for optoelectronic applications. The 9,9´-spirobifluorene (SBF, $C_{25}H_{16}$) molecule consists of two fluorene-like subunits -each composed of two hexagonal rings connected by a pentagonal ring- in a nearly perpendicular configuration. SBF crystallizes in the monoclinic structure, where the individual rings remain planar, but the biphenyl groups of the molecule deviate significantly from planarity due to crystal packing.

In this work, the pressure response of crystalline SBF is studied by Raman spectroscopy, using a diamond anvil cell for pressure generation and Daphne 7474 oil as pressure transmitting medium. With increasing pressure, the Raman peaks shift to higher frequencies, reflecting the bond hardening upon volume contraction, which is much more pronounced for the weaker intermolecular van der Waals interactions than for the stronger intramolecular covalent bonds. The significant changes in the Raman spectrum and the pressure evolution of the Raman peak frequencies at ~1.3 GPa signal a pressure induced structural and molecular conformation transition with a small hysteretic behavior upon pressure release. For $P > 4$ GPa, the reversible decrease of the pressure coefficients of the majority of the intermolecular and some intramolecular peak frequencies indicates another structural modification of the system. A value of ~9 GPa for the bulk modulus of the system at ambient pressure is estimated from the ω-P data for the intermolecular modes in the low-pressure phase. Their pressure coefficients are reduced by ~6 times at 4.2 GPa, indicating that the considerable stiffening of the material in the high-pressure phase emanates from the selective strengthening of the intermolecular interactions.

Topic preference: From Atoms to Devices: growth and fabrication
Presentation preference (oral/poster): Poster
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Rapid bimetallic nanoparticle synthesis using a microfluidic platform

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Keywords: Bimetallic nanostars, microfluidics, SERS

Abstract: Metallic nanoparticles are of great interest in biomedical imaging due to their optical and plasmonic properties. Their potential has been realized for applications in Surface enhanced Raman spectroscopy (SERS) or as contrast agents in magnetic resonance imaging (MRI).[5] The common approach to metal nanoparticle synthesis has been mixing a metal salt with a reducing agent. Bimetallic gold/silver nanoparticles are nanomaterials composed of both gold and silver atoms, often exhibiting unique properties not found in their individual monometallic counterparts.[6],[7] For example, they can have improved catalytic activity, enhanced optical properties (like surface plasmon resonance), and tunable antibacterial activity.[8] Seedless methods are much simpler and offer single-step reactions, but effective mixing is critical for uniform nucleation. [6] Microfluidic devices are ideal for controlling mixing. Such devices are designed to manipulate fluids in channels on the microscale, and have widely been used in various fields (chemistry, biology).[1] Microfluidic devices are often fabricated in polymers such as PDMS or glass.[2] The use of microfluidic devices is more efficient and advantageous over bulk synthesis in terms of reaction yield and improved size, shape distribution and allows precise fluid control and improve heat and mass transfer.[3] Also various shapes of non-spherical particles can be synthesized with microfluidic systems. In these flow systems the nucleation, growth and formation of nanoparticles occur at different designated regions allowing high throughput synthesis with mono-dispersed nanoparticles. In batch synthesis, the nanoparticles are characterized by wider size and shape distribution due to the lack of mixing and separation of particles.[4] By varying the flow rates within the microfluidic device, we can precisely control the reaction kinetics which in turn influences their localized surface plasmon resonance (LSPR) and thus their UV/Vis absorption spectra (Figure 1). In this work, I will present a microfluidic device for bimetallic nanostar synthesis and the use of the synthesized nanostars in acrylamide detection using Surface enhanced Raman spectroscopy (SERS). The advantages of this device: (1) the device enables high efficiency mixing at a wide range of flow rates; (2) allows precise reagent concentration control in a single step for optical property tuning; (3) easy to fabricate using 3D printing. Microfluidic systems demonstrated great potential in the synthesis of organic and inorganic nanoparticles allowing higher quality nanoparticles which are expected to accelerate nanoparticle use in biomedical applications.

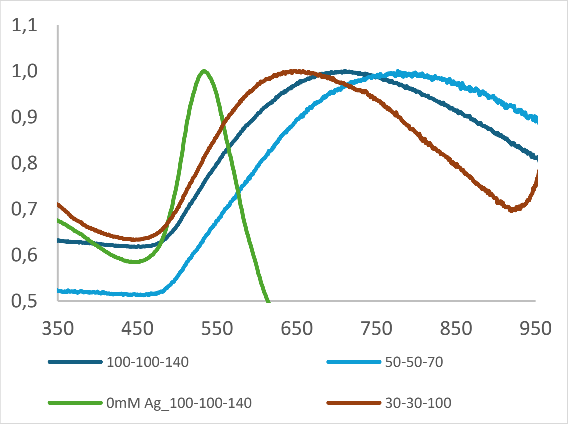

Figure 1. UV–Vis Absorbance Spectra of Gold Nanoparticles synthesized under different flow conditions. Different flow rates of gold ions (1 mM), silver ions (0.2 mM), and ascorbic acid (3 mM) resulted in distinct plasmon resonance peaks. The blue curve (peak ~540 nm) corresponds to spherical nanoparticles, while red-shifted peaks (~630–785 nm) indicate nanostar formation with increased anisotropy. Normalization was applied to compare spectral profiles.

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Deep Learning Models for Biomolecular Systems: The AlphaFold Algorithm

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Abstract: The application of computational modeling, large-scale simulations and artificial intelligence (AI) and machine learning (ML) algorithms in physical systems is an emerging research area. The goal of this work is to provide a computational study of biomolecular systems utilizing both physics-based and data-driven approaches for biomolecular systems. As a representative example the prediction of the 3D structure of proteins from their sequence of amino acids. The AlphaFold algorithm has been recently proposed for predicting a protein's 3D structure from its amino acid sequence [1]. AlphaFold has already achieved higher accuracy than other methods in the prediction of many natural well-folded, globular proteins and a variety of protein complexes, performing particularly well for single chain proteins and extended to predict homomultimers and heteromultimers.

However, many challenges are still remaining regarding the study of more complex protein-based systems, such as the accurate prediction of the 3D structure of intrinsically disordered proteins (IDPs), that are crucial in cellular functions and diseases. Here, we firstly present and then study the applicability of AlphaFold to IDPs. As an example, the method's performance will be assessed on the alpha-synuclein (α-Syn) protein, that when damaged is responsible for Parkinson's syndrome [2]. This includes exploring how the structures derived from AlphaFold can be used together with long-time atomistic molecular dynamics simulations for predicting the structural properties of specific IDPs such as α-Syn under various thermodynamic (temperature and solvent) conditions.

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Partially Reduced Graphene Oxide Biosensor for Protein and Oligonucleotide Detection

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Abstract: Protein and deoxyribonucleic acid (DNA) detection has the potential to contribute to early disease diagnosis and improved patient prognosis. For this reason, the construction of simple and easy to handle biosensors for rapid and accurate monitoring is extremely important. Herein, the necessary steps for the fabrication of a partially reduced graphene oxide (prGO) biosensor are examined. A mild thermal treatment in ambient air to progressively reduce GO drop-casted on a silicon oxide substrate is performed. As a result, the graphene sp^2 lattice is gradually restored and its electrical conductivity is enhanced. At the same time, the prGO retains several functional groups facilitating biomolecular receptor immobilization. Biotinylated bovine serum albumin (b-BSA) and its interaction with fluorescently tagged streptavidin (SA) is used as a model binding reaction to evaluate the efficiency of protein immobilization by fluorescence microscopy. Based on these results, a biosensor is fabricated on Si/SiO_2 substrates comprising the prGO transducer and silver paint contacting electrodes. Resistance measurements confirm that the sensor is capable to detect down to 9 nM of streptavidin through binding to immobilized b-BSA. Finally, in order to demonstrate the health related applicability of the biosensor, a 25 mer DNA strand corresponding to G533C mutation of the RET gene is detected, using a scheme in which the oligonucleotide sequence is tagged with a biotin molecule at its 5' edge, whilst streptavidin is immobilized on the biosensor. Using this approach, DNA concentrations down to 5.5 nM were successfully detected.

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