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Recent results on perovskite nanostructures and heterostructures designed for photovoltaics and quantum light emission

J. Even[1]
[1]*INSA, iFOTON UMR CNRS 6082, University of Rennes, Address, France*

Abstract:

3D halide perovskites are attractive low-cost and solution processed direct band gap semiconductorsfor optoelectronics. The understanding of the excitonic properties, especially its fine structure and the nature of exciton complexes, was questioned with the advent of perovskite nanostructures leading to prospects for quantum light emission. A debate between an initial proposition of a fine structure related to a singlet dark ground state and an inverted dark-bright ordering, was closed recently in favour of the initial proposition. Several open questions are remaining, especially about the nature of the coupling between the charge carriers and the lattice dynamics, which is unusual with respect to classical semiconductors. Direct experimental investigations on the low energy lattice dynamics including neutron scattering will be presented, together with state of the art atomistic simulations of the lattice dynamics and electron-phonon coupling. The regime of low-temperature Fröhlich polaronic coupling in bulk 3D perovskites and quantum dots is also explored. 2D multilayered perovskites introduced by Calabrese in 1991 share similarities with 3D perovskites. Calabrese's Ruddlesden-Popper phases were completed more recently by "Alternative cations in the interlayer" and Dion-Jacobson phases, leading to a consistent classification of multilayered perovskites. Exploring the potential of 2D perovskites for PV and the association of 2D and 3D perovskites in solar cell architectures is a long-term joint project with colleagues in US that started years ago including the first breakthrough on 2D perovskite for PV (Tsai Nature 2016). Combined in 2D/3D bilayer structures using new versatile growth methods, excellent solar cell device stability can be achieved. Band alignment calculations nicely explain the difference of performances for ni-p or p-i-n devices. Our lattice mismatch concept provides further guidance for the choice of the proper 2D/3D combinations, leading to enhanced stability for FAPbI3-based solar cells published in 2024 in Science.

Cluster Crystals: from a theorist's toy model to experimental realization

Christos N. Likos
Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria

Abstract: Crystals are orderly states of matter in which particles with sizes ranging from sub-nanometer to micron are arranged in a periodic lattice. Crystalline solids epitomize the notion of rigidity, lying at the antipode of fluidity that is embodied by liquids. Accordingly, hybrid, exotic phases that combine crystallinity with (super-)fluidity have fascinated researchers both in the classical realm of soft matter physics and in the quantum domain. In usual crystals, the lattice constant a and the particle concentration c obey the proportionality $a \propto c^{-1/3}$, dictated by the condition that the (conventional) unit cell be populated by a fixed number of particles determined by the lattice geometry. Cluster crystals, a newer concept, are unconventional states of matter whose lattice sites are occupied by clusters of fully or partially overlapping particles rather than single ones. In these states, the number of overlapping particles within a cluster, the lattice-site occupancy N_{occ}, is a fluctuating quantity, with its expectation value scaling with concentration as $N_{\mathrm{occ}} \propto c$ and thus resulting in a concentration-independent lattice constant, the latter being the salient structural characteristic of both cluster crystals and cluster quasicrystals.

In this talk, I will briefly review 20 years of theoretical work that led to a recent, theory-informed, experimental discovery of this new state of matter.

Stretching elasticity of bistable linear polymers and loops

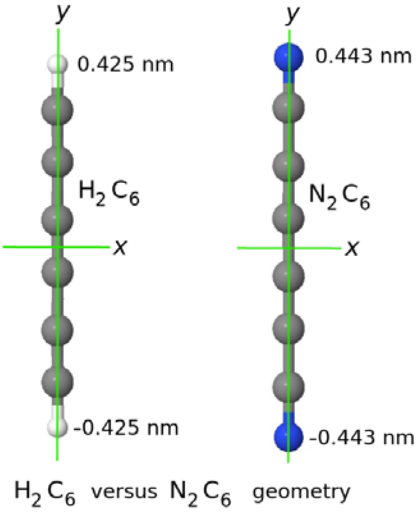
P. Benetatos
Department of Physics, Kyungpook National University, Daegu 41566, Republic of Korea

Abstract: The local bending stiffness of semiflexible polymers may fluctuate due to internal conformational changes (e.g, the helix-coil transition in polypeptides or the thermal denaturation of double-stranded DNA) or due to the reversible attachment/detachment of ligands from the environment (e.g., DNA-binding proteins or hybridization of oligomers). We theoretically analyze the tensile elasticity of a strongly-stretched wormlike chain consisting of N bistable blocks. The bending stiffness of each block is an annealed degree of freedom with two values. We calculate the force-extension relation of this chain in both the fixed-force (Gibbs) and the fixed-extension (Helmholtz) ensemble. We show that, for finite N, there is significant ensemble inequivalence. Under certain conditions, in the Helmholtz ensemble, the tensile compliance becomes negative. (PB, J. Chem. Phys. 157, 2022.) We also consider a rod-like wormlike chain with fluctuating bending stiffness grafted at an angle to a rigid substrate subject to a force at the other end. We show the emergence, under certain conditions, of compliance higher than that corresponding to the two values of the bending stiffness (Gibbs ensemble), as well as negative compliance (Helmholtz ensemble). (M. Razbin and PB, Polymers 15(10), 2023.) In addition, we are going to present an analysis of flexible polymer loops under tension, undergoing reversible transitions between two states: looped and unlooped, or looped and zipped. In the case of a reversible necklace (concatenated reversible loops and zipped chains in the thermodynamic limit) under tension, using the generating function method, we show that the flexibility of the zipped part has a significant effect on the force-temperature phase diagram (G. Noh and PB, Phys. Rev. E, in press).

Oxidation dynamics in polyynes and dicyanopolyynes

L. Chalkopiadis, K. Lambropoulos C. Simserides
Department of Physics, National and Kapodistrian University of Athens, Panepistimiopolis,
Zografos GR-15784, Athens, Greece

Abstract: Femtosecond to attosecond spectroscopy permits now the study of really fast carrier dynamics [1-5], in particular, the spatial and temporal charge density evolution, after an initial oxidation or reduction. We study such processes in molecular atom-thick wires: polyynes and dicyanopolyynes (depicted in the scheme below). These are straight symmetric molecules containing carbon and hydrogen or nitrogen, respectively. We derive the electronic structure and focus on hole transfer in the first members of the series of polyynic carbynes and dicyanopolyynes, which have length of the order of nanometer. We use methods based on density functional theory (DFT), including constrained DFT (CDFT), time-dependent DFT (TDDFT) and real-time TDDFT (RT-TDDFT), with Löwdin population analysis. We also develop a Tight Binding (TB) variant using all valence orbitals of all atoms and use it for the same purposes. We calculate the electronic structure, the time-dependent dipole moment and the probability to find the carrier at each site, their mean over time values, the mean transfer rates from the oxidation site to other sites and the frequency content or carrier movement, analysing charge and dipole moment oscillations. We compare the static case with the case including zero-point motion. The initial conditions for RT-TDDFT are defined by CDFT, while in TB, we let different initial conditions: we can place the hole at any particular orbital or distribute it among a number of orbitals; it is also possible to include phase differences between orbitals. We compare with available experimental results. This is a freshly submitted work [7].



H_2C_6 versus N_2C_6 geometry

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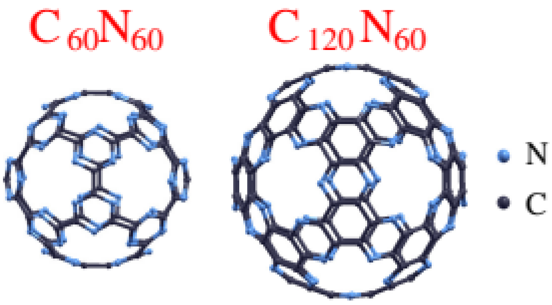
Porous carbon nitride fullerenes: a DFT study on a novel family of porous cage molecules

Z. G. Fthenakis[1,2,3], N. N. Lathiotakis[1]
[1] *Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, GR-11635, Athens, Greece*
[2] *Ististuto Nanoscienze del Consiglio Nazionale delle Ricerche (CNR-NANO), IT-56127, Pisa, Italy*
[3] *National Enterprise for nanoScience and nanoTechnology (NEST), Scuola Normale Superiore, IT-56127, Pisa, Italy*

Abstract: The fact that fullerenes are the 0-dimension (0D) counterparts of graphene, gives rise to a reasonable question, of whether similar 0D counterparts of the 2-dimensional (2D) porous graphitic carbon nitrides (g-C_nN_ms) exist. Here, we demonstrate that these 0D structures, which we call Porous Carbon Nitride Fullerenes exist and we study theoretically the first two members, ($C_{60}N_{60}$ and $C_{120}N_{60}$), of that family.

Porous g-C_nN_ms are 2D structures, formed from a periodic porous graphene lattice, substituting the 2-fold coordinated C atoms at the pore edges and maybe some other 3-fold coordinated, with N atoms. Members of this family of structures have been synthesized and they have a broad spectrum of interesting applications in catalysis, gas separation, water desalination, hydrogen storage, Li-ion batteries, etc. Therefore, it will not be surprising if these properties are inherited by their 0D counterpart fullerenes, which will also have additional interesting properties rising from their cage geometry.

Utilizing DFT calculations with state-of-the-art functionals, we study the stability and the structural, electronic, and vibrational properties of $C_{60}N_{60}$ and $C_{120}N_{60}$ and we compare them with those of C_{60}. The optimizations and the vibrational analysis reveal that these molecules are dynamically stable. The HOMO-LUMO gap was found to be large, and the structure exhibits aromatic character. Performing optimization calculations for their positive and negative ions, their ionization potential and electron affinity were also found. Their formation energy, with respect to their 2D counterparts g-CN and g-C_2N, respectively was found to be less than 0.1 eV/atom. Moreover, using NVT molecular dynamics simulations with two ReaxFFs (CHON-2019 and GR-RDX-2021), we found that $C_{60}N_{60}$ and $C_{120}N_{60}$ are thermally stable at temperatures well above 1000 and 2000 K, respectively. With these properties, the new proposed molecules are expected to be of great importance after their synthesis.



Acknowledgements:
ZGF acknowledges financial support from the project PRIN 2022 - Cod. 202278NHAM (PE11) CHERICH-C "Chemical and electrochemical energy storage materials from organic wastes: the treasure hidden in C-based materials" - CUP B53D23008590006, funded by the European Union – Next Generation EU in the context of the Italian National Recovery and Resilience Plan, Mission 4, Component 2, Investment 1.1, “Fondo per il Programma Nazionale di Ricerca e Progetti di Rilevante Interesse Nazionale (PRIN)”.

Superlubricity of graphene and 2D materials

C. Androulidakis[1], G. Fanourgakis[2], C.S. Garoufalis[3], E. Papasouli[2], E.N. Koukaras[2]
[1]Prometheus Division of Skeletal Tissue Engineering, KU Leuven, O&N1, Herestraat 49, PB 813, 3000 Leuven, Belgium
[1]Skeletal Biology and Engineering Research, KU Leuven, ON1 Herestraat 49, PB 813, 3000 Leuven, Belgium
[2]Laboratory of Quantum and Computational Chemistry, Aristotle University of Thessaloniki, Thessaloniki, 54124, Greece
[3]Materials Science Department, University of Patras, 26504 Patras, Greece

Abstract: Superlubricity is a kinetic state in which friction becomes negligible or even vanishes. The superlubric state can arise when incommensurate contacts are formed between periodic interfaces, such as 2D crystal materials. Here we show our recent findings that superlubricity can manifest at the mm scale by removal of stick–slip instabilities through application of strain. Effectively, we examine the novel notion of manipulating superlubricity in 2D materials by mechanical straining and manipulation of morphology.

The approach followed vastly differs from existing methodologies, is based on non-invasive Raman-based techniques rather than AFM-based that considerably affect the samples. We shall discuss results from graphene–graphene interface. By applying strain, we tune the frictional behaviour and achieve superlubric behaviour. We expand the concepts and procedures to heterostructures of different 2D crystal combinations. We combine theory and experiment for an in-depth treatment of the manifestation of superlubricity in 2D homo- and hetero-structured materials, much required for both macroscopic and microscopic applications.

2D heterostructures are emerging as a most exciting class of 2D materials that seem to exhibit mechanical and electronic properties far richer than their constituents.

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Growth of Large-Area Tungsten Disulfide Via Sodium-Mediated Chemical Vapor Deposition

D. Maratos[1,4], N. Balakeras[2], A. Michail[1,3], K. Filintoglou[5], V. Tagoulis[4], K. Papagelis[1,2] and J. Parthenios[1]
[1] *Institute of Chemical Engineering Sciences, FORTH/ ICE-HT, Patras 26504, Greece*
[2] *School of Physics, Department of Solid-State Physics, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece*
[3] *Department of Physics, University of Patras, Patras 26504, Greece*
[4] *Department of Chemistry, University of Patras, Patras 26504, Greece*
[5] *HENANOTEC, Komninon 17, 54 624, Thessaloniki, Greece*

Monolayer tungsten disulfide (WS_2) is a promising semiconductor material with significant potential in optoelectronic applications. Among various 2D materials, Chemical Vapor Deposition (CVD) has emerged as the most efficient method for producing single and few-layered WS_2. Previous research has demonstrated large-area growth of molybdenum disulfide (MoS2) using aqueous solutions of Na_2WO_4 as wet precursors. Additionally, it has been observed that factors such as strain and doping considerably influence the material's properties, subsequently impacting its practical applications.

In this study, we introduce a novel approach for producing single and few-layered WS_2 crystals on a Si/SiO_2 substrate. Our method employs a sodium-mediated process, using either NaCl as a promoter or NaS as an additional chalcogen precursor. The experimental procedures involve a meticulous CVD process where these sodium compounds are blended on the Si/SiO2 substrate to enhance the growth quality of WS_2 crystals.

To analyze the properties of the synthesized crystals, we utilized micro-Raman and micro-Photoluminescence (PL) spectroscopy. These techniques allowed us to investigate the effects of doping and strain introduced during the CVD process. By conducting a correlative analysis of the spectroscopic data alongside Raman and PL imaging, we aimed to reconstruct the nucleation steps to gain a deeper understanding of the crystallization mechanism.

Our findings provide insights into the stoichiometry, deposition procedures, and other experimental conditions crucial for high-quality, bottom-up production of WS_2. The study discusses the impact of different precursors on the growth process and the resultant material characteristics. This comprehensive analysis contributes to the optimization of CVD parameters, facilitating the advancement of WS_2-based applications in the field of 2D materials.

In Situ Observation of GaAs Nanowire Growth : Focus on the Crystal Phase Dependence on the Physical State of the Catalyst

V. Sallet[1], G. Patriarche[2], L. Travers[2], F. Glas[2], J.-C. Harmand[2]
[1]*GEMAC, Université Paris-Saclay, CNRS, Université de Versailles St Quentin en Yvelines,*
45 avenue des Etats-Unis, 78035 Versailles cedex, France
[2]*Centre de Nanosciences et de Nanotechnologies (C2N), Université Paris-Saclay, CNRS,*
10 Boulevard Thomas Gobert, 91120 Palaiseau, France

Abstract: Crystal-phase heterostructures alternating different phases in the same material, e.g. crystal-phase quantum dots with perfectly abrupt interfaces, could be fabricated by an accurate control the catalyzed-growth conditions (temperature, droplet contact angles, source fluxes…). This arouses a strong interest for the next generation of electronic and photonic devices.

In this study, the fabrication of GaAs NWs has been investigated in real time using NANOMAX facility, a modified FEI environmental transmission electron microscope, where two molecular beam sources have been implemented to supply Ga and As$_4$ fluxes towards a heated SiC membrane. Gold-gallium alloy droplets were formed to act as catalysts. In particular, we distinguished and compared two growth mechanisms : VLS mode (vapor-liquid-solid) where the catalyst droplet is liquid, and VSS mode (vapor-solid-solid) where it is solid. In such *in situ* observations, not only the construction, plane by plane, of the GaAs crystal structure is followed, but also the phase and composition of the Au$_{1-x}$Ga$_x$ catalyst can be determined in the case of VSS mode. That enables to precise where the catalyzed growth takes place in the Au-Ga phase diagram. Commonly in the literature, the VSS growth is achieved by lowering the SiC membrane temperature (i.e. crossing the Au-Ga liquidus line vertically). Interestingly in this work, when the growth occurs close to the AuGa$_2$ solidification point, we show that the physical state of the catalyst (liquid, solid, or mixed) can be also tuned by varying the Ga composition in the droplet (i.e. crossing the Au-Ga liquidus line horizontally). This was achieved by opening the As flux which involved a consumption of the Ga in the catalyst, or closing it in order to refill the droplet with Ga. As a result, playing with the As flux at constant temperature, we demonstrate that we can master a growth cycle which alternates cubic and hexagonal phase GaAs segments, as illustrated in figure 1. These studies help to understand the growth mechanisms for a better control of crystal-phase heterostructures in semiconductor nanowires.

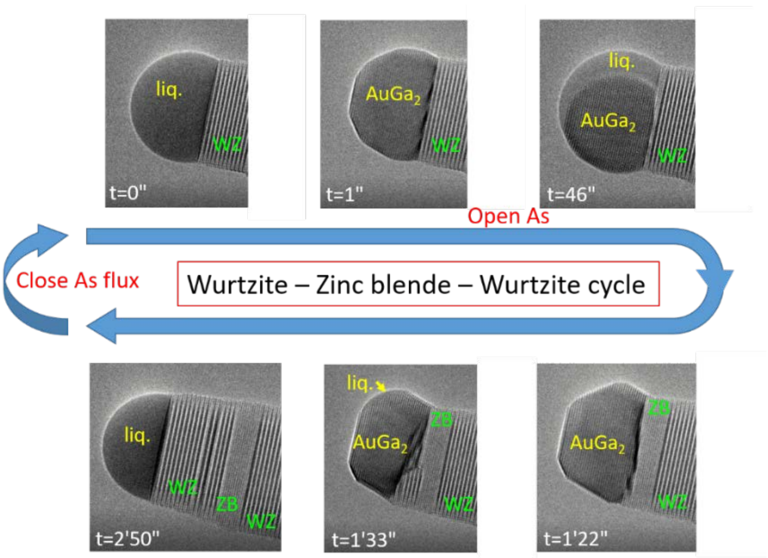

Fig.1. Transmission electron microscopy images from in situ observations, illustrating the growth of hexagonal or cubic phase GaAs NW.

An empirical model for epitaxial semiconductor superlattices

K. Pantzas[1], V. Trinité[2], A. Vasanelli[3], G. Beaudoin[1], C. Sirtori[3], I. Sagnes[1] and G. Patriarche[1]
[1]Centre de Nanosciences et de Nanotechnologies, CNRS Université Paris Sacley, 91120, Palaiseau, France
[2]III-V Lab, 91767, Palaiseau, France
[3] Laboratoire de Physique de l'École Normale Supérieure, ENS, Université, PSL, CNRS, Sorbonne Université, Université de Paris, 75005 Paris, France

Abstract: An empirical model for epitaxial superlattices is proposed. The model is built from atomically resolved chemical mappings of InGaAs/InAlAs superlattices, obtained from quantified high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) micrographs [1]. The model accounts for discrepancies in composition, well and barrier width, and interface roughness. Once calibrated, it is used to predict transitions in InGaAs/InAlAs asymmetric couple quantum-well structures. Compared to an ideally abrupt potential, this model is shown to predict optical transition energies within 1meV of the transition energies measured using multi-pass absorption measurements, opening the path for predictive simulation of quantum cascade devices.

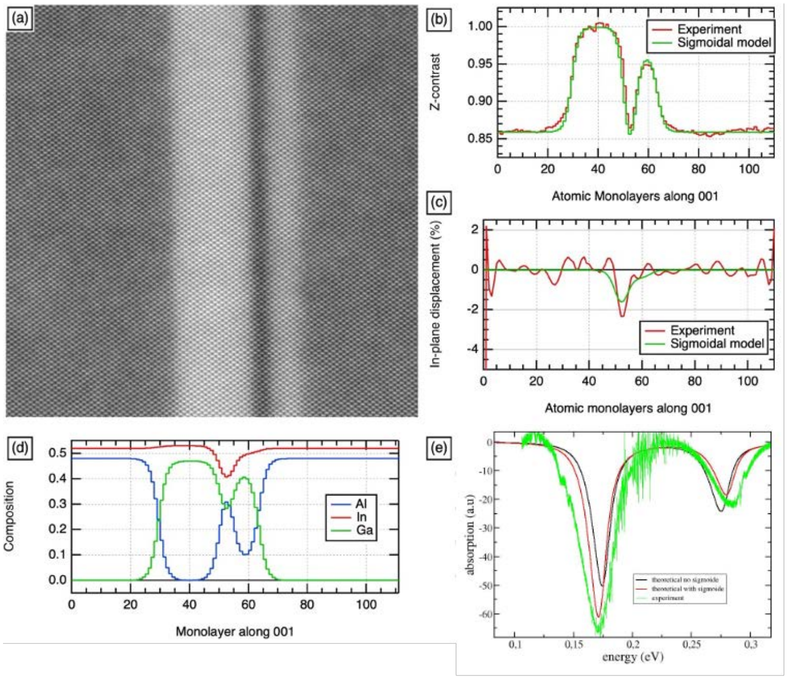

Figure: (a) HAADF-STEM image of an InGaAs/InAlAs asymetric coupled quantum well structure; (b) Experimental Z-contrast and fit obtained using the sigmoidal model; (c) Measured out-of-plane displacement and fit based on sigmoidal model; (d) Fitted compositions for In, Al, and Ga; (e) Measured and fitted absorption spectra.

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High Quality Ordered & Tunable Size Nanostructures of Titanium Nitride for Plasmonic Applications

S. Kassavetis, P. Rampota, S. Panos, N. Pliatsikas, D. Tselekidou and P. Patsalas
Nanotechnology Lab LTFN, Physics Department, Aristotle University of Thessaloniki, Thessaloniki GR-54124, Greece

Abstract: Novel and cost-efficient fabrication techniques of alternative plasmonic nanostructures pave the pathway for practical applications in various fields such energy harvesting, photonics, microelectronics and medicine. Transition metals nitrides (TMNs) emerge as alternative plasmonic nanomaterials suitable for a wide range of applications from photovoltaics to photonics and medicine. The TMNs are conductive ceramics that combine exceptional properties such as substantial electronic conductivity, high melting point (>3000 K) and tunable work function, while the TMNs are particularly stable in hostile chemical environments, high temperature, and strong electric fields, such as in lasers. Among them, Titanium Nitride (TiN) is emerging as significant candidate material for plasmonic applications and in this work, we focus on the low-cost fabrication of TiN nanostructures with controlled spacing and tunable dimensions using a combination of Nanosphere Lithography (NSL) and several reactive magnetron sputtering (MS) deposition techniques such as DC, Closed-Field Unbalanced MS or Highly Power Impulse MS (HIPMS). NSL appears as a very promising approach, due to its rapid implementation and compatibility with wafer-scale processes. A suspension of monodisperse polystyrene nanospheres (diameter, d=552 nm or d=175 nm) was spin-coated on a substrate (such as Si (001), glass, flexible PET) to form the colloidal mask.

Subsequently, the selective growth of TiN was made by the above mentioned MS in Ar/N atmosphere, while the MS process parameters were also fine-tuned to increase the directionality of deposited species, and the TiN crystal quality (low concentration of point defects). Their morphology and the quality are evaluated using Atomic Force Microscopy that showed the fabrication of tailorable highly ordered TiN nanostructures by varying the thickness 10-30 nm (controlled by deposition time), size (by using nanospheres with different diameter) and shape (by angular MS deposition) such as nanotriangles, nanorods, nanorod rings, and nanowire arrays.

Ultrafast spin currents and applications

Evangelos Papaioannou[1]
[1]*Department of Physics, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece*

Abstract: The fascinating field of ultrafast spin physics combines spintronics with optics, microwaves and ultrafast photonics. The effects of spin current generation and transport hold the promise for novel research directions in physics paving the way for applications in engineering and information technologies. In this presentation we will ask ourselves first of all what is a spin current and what are its properties. We will then address the different ways to generate, transport and manipulate ultrafast spin currents.

Furthermore, the focus will not only be on the physical properties of spin currents but also on applications. Among others we will see how spin currents have entered the field of THz physics [1]. The need for controllable spin current properties for efficient THz emission from spintronic structures is emerging. The key factor that defines the strength of the THz emission is the transfer of the spin current across the spintronic layers and its conversion to a charge current. We will watch how this can take place by addressing results from magnetic-based multilayers having alloys like FePt, and antiferromagnets as layers with different structural and magnetic anisotropies [2,3]. In a next step, we will show how the spin and the subsequent charge current dynamics can shape the THz bandwidth and signal strength.

Spin currents hold nowadays the promise for new applications as for example in the field of THz technologies since they are able to provide high field strengths, spatiotemporal modulation of the THz beam and a very wide spectrum reaching up to 30 THz [1].

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Design principles for the development of high frequency (>3 MHz) MnZn-ferrites

G. Kogias[2], I. Tsoukalas[1], S. Zaspalis[1,2], V. Tsakaloudi[2], S. Papaioannou[2], D. Holz[3], E. Rauchenwald[4], V. Zaspalis[1,2],

[1]Laboratory of Materials Technology, Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki, Greece

[2]Laboratory of Inorganic Materials, Chemical Process and Energy Resources Institute, Center for Research and Technology-Hellas, Thessaloniki, Greece

[3]Ferroxcube-Yageo Europe Corporation, Skiernewice 96-100, Poland

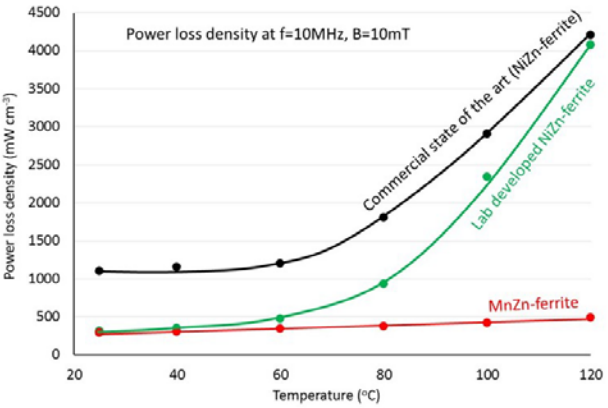
[4]Huawei Technologies Austria GmbH, A-1120, Vienna, Austria

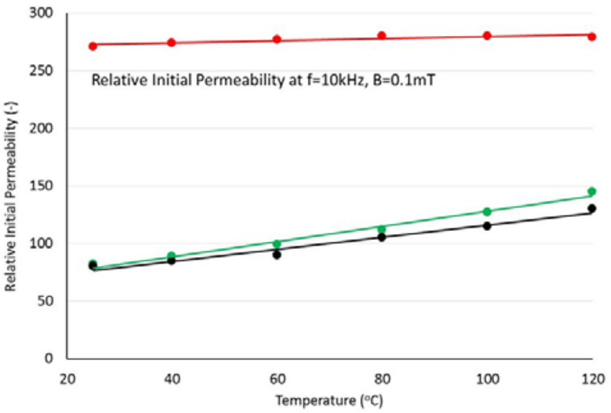
Abstract:

The tendency towards device and component miniaturization, the continuously increased operation frequencies and the emerged wide band and high switching frequency semiconductors require ferrites with very good performance at frequencies within the MHz range and high temperatures. Consequently, high frequency MnZn-ferrites form the most important trend in nowadays research and development efforts towards new MnZn ferrite materials. However, the application frequency of MnZn-ferrites is limited up to frequencies of 1-3 MHz and no commercially available materials exist for higher frequency applications that require low power loss densities.

Power loss analysis at frequencies up to 10 MHz indicated that the development of high frequency polycrystalline materials passes primary through reduction of ferromagnetic resonance (mainly spin resonance) losses and secondary through reduction of eddy current losses while the strongly composition dependent hysteresis losses can be considered negligible.

Based on these recognitions polycrystalline MnZn-ferrite materials have been developed with superior power loss densities at frequencies up to 10 MHz, quite better than currently commercially available or developed NiZn-ferrites at this frequency range (see Figure below). As it will be described in this presentation, the improvements are achieved by **i**) increasing the magnetocrystalline anisotropy with the usage of highly anisotropic cations **ii**) creating relatively dense fine grained microstructures at low sintering temperatures (i.e. 1175°C) and **iii**) using relatively high oxygen partial pressures in order to enable selective oxidation of the grain boundaries.





Magnetic steel health monitoring in the nano-scale

Xenia Vourna[1], Aphrodite Ktena[2], Evangelos Hristoforou[1]
[1]Laboratory of Electronic Sensors, School of Electrical and Computer Engineering, National TU of Athens, Zografou Campus, Athens 15780, Greece
[2]National and Kapodistrian University of Athens

Abstract: The aim of the current work is to demonstrate the ability of determining the number, density and distribution of dislocations and nano-precipitations in steels. Magnetization process is evidently dependent on the microstructure of the magnetic substance. The presence of dislocations and nano-precipitates affects both magnetic domain wall mobility and magnetic domain rotation. Thus, the B-H loops, the Barkhausen noise, the magnetoacoustic emission and the surface magnetic permeability of steels are modified with the level of plastic deformation, the presence of sub-grains in the grain, as well as the size and distribution of nano-precipitates in the grain. These four types of magnetic measurements are in agreement with microstructural changes observed mainly by electron back scattering diffraction (EBSD), but also with transmission electron microscopy (TEM) and XRD based stress tensor analysis. The dependence of the magnetic properties change on the microstructure is modeled with respect to the dependence of domain wall motion and domain rotation on dislocations and nano-precipitates. A typical dependence of the crystalline mis-orientation angle in a grain on the coercive field is illustrated in Figure 1, while Figure 2 shows the agreement in the increase of the Barkhausen noise with the Vicker’s hardness, thus allowing for a magnetic non destructive determination of hardness in steels. As a result of the whole magnetic procedure, one may use the above mentioned magnetic techniques in order to determine the level of plastic deformation of steels, in other words the nano-cracks of steels, thus improving significantly the existing state of the art in steel non-destructive testing and offering the possibility of early stage steel health monitoring.

Novel Hybrid Ferromagnetic Fe-Ni Nanoalloys Grown on Nanodiamonds

Panagiotis G. Ziogas, Athanasios B. Bourlinos and Alexios P. Douvalis

Physics Department, University of Ioannina, 45110 Ioannina, Greece

This work presents a novel hybrid nanostructured magnetic material consisting of ferromagnetic (FM) fcc Fe-Ni nanoparticles (NPs) grown on nanodiamonds (NDs) nanotemplates. The development of this hybrid magnetic nanomaterial is realized through combination of wet chemistry and thermal annealing under vacuum. The characterization and study of the prepared samples reveal that the thermal annealing of the as-made Fe-Ni-oxide/NDs hybrid precursor under a range of annealing conditions leads to the development of metallic Fe-Ni alloy NPs, averaging 10 nm in size and exhibiting uniform distribution on the NDs nanotemplates. These alloy NPs have a predominant nickel content of approximately 66 at. %, and demonstrate FM behavior throughout a temperature range from 2 K to 400 K, with maximum magnetization values ranging between 8.6 and 10.9 emu/g and coercivities ranging between 10 and 490 Oe. Moreover, ^{57}Fe Mössbauer spectroscopy reveals that apart from the predominant fcc $FeNi_3$ phase, iron atoms participate also in the formation of a tetragonally distorted martensitic-type Fe-Ni phase within the alloy NPs, while residual inherent Fe-Ni-oxide precursor seed NPs are also present. The development of this distinctive martensitic-type phase is attributed to the diffusion of carbon atoms originating from the NDs' surfaces within the Fe-Ni NPs lattice during its formation at elevated temperatures. This comes as a consequence of the unique morphological properties of the NDs growth matrices, which facilitate surface formations and reconstructions of sp^2 nanostructures. Apart from their diffusion within the Fe-Ni NP lattice, the carbon atoms are also constructing layered graphitic-type nanostructures enveloping the metallic alloy NPs (Figure 1). These non-typical nanohybrid materials, reported here for the first time in the literature, hold significant potential for use in applications related, but not limited to, biomedicine, biopharmaceutics, catalysis, and other various contemporary technological fields.

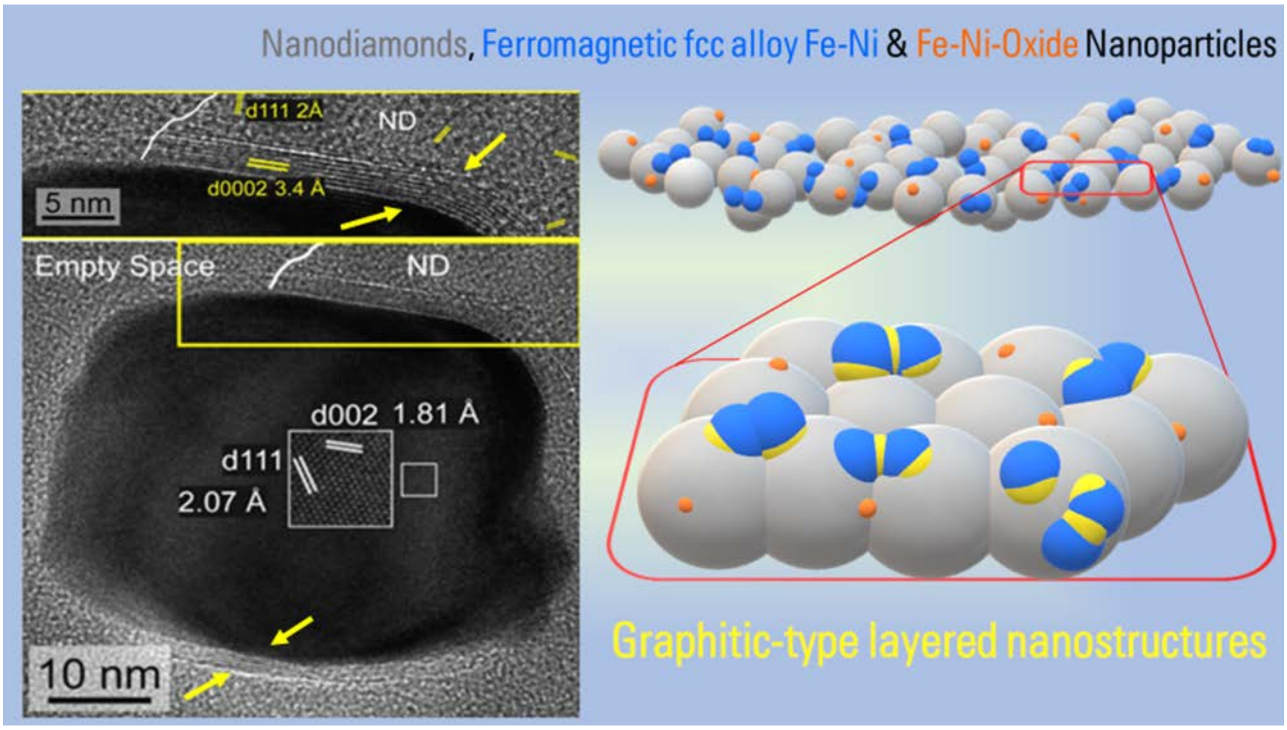


Figure 1. Schematic representation of metallic Fe-Ni alloy NPs (coloured blue) grown on the surfaces of a ND nanotemplate (coloured grey), along with residual precursor Fe-Ni-oxide NPs (coloured orange-right). In the interface between the NDs and metallic NPs the carbon atoms construct layered graphitic-type nanostructures (shown with yellow arrows in the HRTEM image-left).

Development of magnetic powders for inductive heating

V. Tsakaloudi[1], S. Papaioannou[1], V. Zaspalis[1,2]
[1]Laboratory of Inorganic Materials, Chemical Processes and Energy Resources Institute, Centre for Research and Technology-Hellas (CERTH), 57001 Thermi-Thessaloniki, Greece
[2]Laboratory of Materials Technology, Department of Chemical Engineering, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

Abstract:

The interest in the heating capabilities of magnetic materials has arisen in recent years, aiming to assist in the design of thermally activated processes and applications. Under this scope, the present work deals with the investigation of the inductive behaviour of conventional polycrystalline ferrite materials and the development of the respective inductive ferrite powders to be used as heating agents in chemical reactors, considering that at the micro range, the ferrite particles are multidomain, exhibiting intraparticle domain walls. The primary goal being to correlate the magnetic performance between the sintered core state and the powder state, Mn-Zn ferrite materials of the general formula ($Mn_x Zn_{1-x} Fe_2O_4$), x=0, 0.2, 0.4, and Mg-Mn ferrite materials of the general formula ($Mg_y Mn_{1-y} Fe_2O_4$), y=0, 0.2, 0.4 and 0.6 were prepared following the solid-state reaction method. After mixing, prefiring and milling at optimal process conditions for each ferrite group, the granulated powders were sintered in appropriate atmosphere-controlled conditions, either in the state of compacted toroids or free-standing granulate. The magnetic performance of the sintered toroids was evaluated via initial permeability, saturation magnetization and BH loop measurements, while their structural and morphological characteristics were also determined. The BH loops of the sintered granulate were obtained via VSM tests, accompanied by the respective structural and morphological investigation. The heating ability of the magnetic materials was evaluated on an in-house built-up module. A direct correlation between the loss performance of the sintered core and the sintered granulate is revealed. At the same time, the crucial role of the chemical, structural and morphological parameters involved in the matrix is highlighted. Optimization paths towards the enhancement of the heating ability on the best-performing carriers are proposed.

1. Controlling the properties of magnesium-manganese ferrites, M.Singh, S. P. Sud, *Materials Science and Engineering: B,* 83, 1-3 (2001) 180-184
2. Selection of ferrite powder for thermal coagulation therapy with alternating magnetic field, T. Maehara et al, *Journal of materials Science* 40 (2005) 135-138

Magnetic fluctuations in strongly correlated systems: from toy models to realistic materials simulations

M. Chatzieleftheriou[1], S. Biermann[2], E. A. Stepanov[3]
[1] *CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France*

Abstract: Strongly correlated electronic systems exhibit intriguing properties and highly complex phase diagrams, including metal-to-insulator transitions, magnetic/charge orderings and the field’s holy grail: high temperature superconductivity. Their theoretical description is very challenging and various many-body methods have been developed to this direction. I will present results using state-of-the-art numerical techniques that allow for an accurate description of both strong local electronic correlations and spatial fluctuations. I will discuss the application of this approach on the study of a simple model, relevant for a series of materials, where we have analyzed the interplay of Mott physics and magnetic fluctuations [1]. We have identified the Slater and Heisenberg regimes in the phase diagram, which are separated by a crossover region of competing spatial and local electronic correlations. This bridging of the two limits (the spin-fluctuation-dominated Slater regime at weak coupling and the Mott insulator at strong-coupling) had been a key missing ingredient to our understanding of metal-insulator transitions in real materials. I will, moreover, present results of a recent work on the perovskite Sr_2RuO_4 compound, where we have performed realistic calculations and have accurately reproduced the experimentally estimated magnetic susceptibility, resolving a long-standing discrepancy, in the community, between theory and experiment.

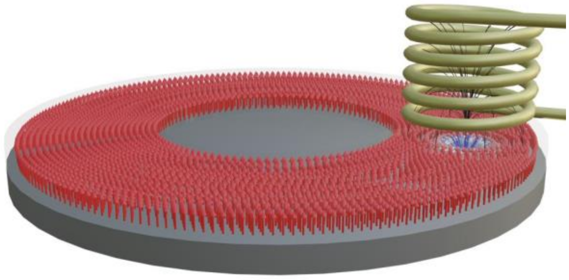
[1] M. Chatzieleftheriou, S. Biermann, E. A. Stepanov, PRL 132, 236504 (2024)

Magnetic skyrmions in nanorings for electric pulse generation

Dimitris Kechrakos

Physics Laboratory, Department of Education, School of Pedagogical and Technological Education (ASPETE), 15122 Heraklion Attikis, Greece

Abstract: Magnetic skyrmions are spatially localised whirling configurations of the magnetization that hold promises as novel information carriers in modern spintronics devices. Here, we study skyrmion-based ring-shaped nanoscale devices by means of micromagnetic simulations and analytical calculations. In the first part, we demonstrate three application scenarios of ferromagnetic nanorings [1] for electrical pulse generation, namely a “clock” with tuneable frequency, an alternator based on engineered anisotropy gradient, and an energy harvester exploiting existing thermal gradients. We show how to precisely tune the frequency and amplitude of the output electrical signals by varying the material parameters, the sample geometrical parameters, the number of skyrmions, and we examine the device functionality under realistic conditions of temperature and material defects. In the second part, we improve the previous concepts by implementing synthetic antiferromagnet (SAF) nanorings [2], that supress the detrimental Skyrmion Hall Effect and can be efficiently downscaled while they can support higher skyrmion velocities. As an outcome, generated electrical pulses in the GHz regime become feasible in SAF nanorings. Furthermore, skyrmions are shown to exhibit comparable performance to Neel domain walls in SAF nanorings as long as their mutual repulsions remain weak. Finally, we introduce a novel skyrmionic three-phase AC alternator based on a SAF nanoring, which operates in the GHz regime and demonstrate an optimized functionality approach.



Energy Harvesting by a gradient-driven skyrmion and a Faraday coil.

We acknowledge financial support by the Special Account for Research of ASPETE through program *“Strengthening of Research in* ASPETE”.

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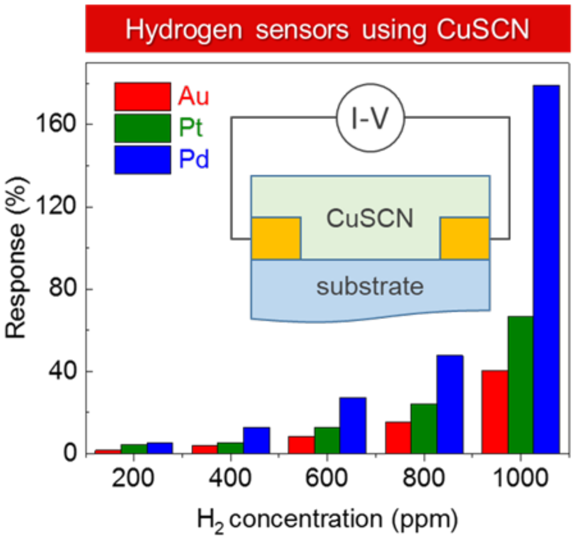
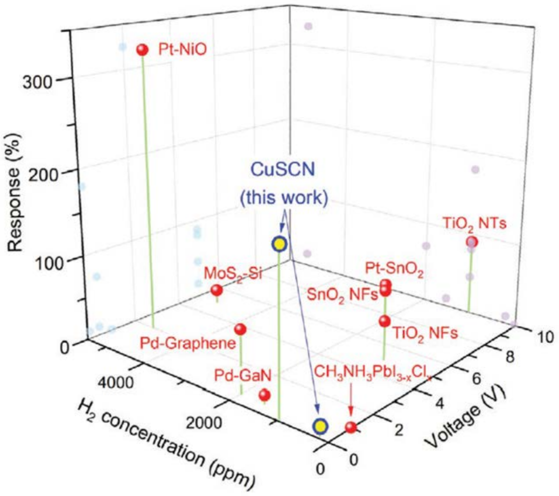
[2] D. Kechrakos, et al, J. Phys. D: Applied Physics (2024) (to appear)

Low power conductometric Gas sensors based on p-type Semiconductors

V. Binas[1,2]
[1]Foundation of Research and Technology - Hellas, Institute of Electronic Structure & Laser (FORTH-IESL),Heraklion, Greece
[2] Department of Chemistry, Aristotle University of Thessaloniki, Greece

Metal oxides have been used widely as the gas sensing element in solid-state devices due to their sensitivity toward various atmospheric elements. However, the often high working temperature combined with the high power consumption that is required to operate such sensors represent two major technical and scientific challenges. For the past 50 years a broad range of metal oxides (e.g., SnO2, ZnO, In2O3, Cu2O, CuO, NiO, TiO2) [1] have been studied for the detection of toxic and hazardous gases such as O3, NOx, CO, CO2, VOCs, CH4, H2. [2–3] Among them, various metal oxides semiconductors, such as n-type SnO2, ZnO, TiO2, and p-type CuO, NiO, have been reported to be sensitive, yet only a handful of these sensors were shown to operate at room temperature reversibly while consuming low power. In this talk I will give an overview of my research on low power conductometric gas sensors based on ultrathin p-type semiconductors (such as metal thyocyanates, cobalt vanadates etc).





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Single-layer multifunctional materials with humidity driven mobility

I. Tzoumani[1], D. Druvari[1], K. Andrikopoulos[1], J.K. Kallitsis[1,2]
[1]*Department of Chemistry, University of Patras, GR-26504 Rio-Patras, Greece*
[2]*Institute of Chemical Engineering Sciences, FORTH/ICE-HT, GR-26504 Rio-Patras, Greece*

Abstract:

A novel class of smart responsive actuators has been developed, capable of converting environmental stimulus like humidity to reversible mechanical motions. These advancements have significant applications in cutting-edge fields like soft robotics and smart switches. Humidity-driven actuators have received considerable research interest due to the environmentally friendly and widely available nature of water. The design principles for humidity-driven actuation typically involve inducing asymmetric deformation by differentially swelling or deswelling materials with varying hydrophilic properties in response to humidity changes or by having the same material respond to a humidity gradient.

In this study, we introduce single-layer crosslinked membranes that show high sensitivity to humidity[1-3]. These hybrid membranes are prepared in environmentally friendly solvents like ethanol and even water in some cases[3]. The fabrication processes are cost-effective, scalable, and environmentally friendly. The developed membranes were analysed for their microstructure morphology, physicochemical, and mechanical properties, antimicrobial properties and an extensive study was conducted on their humidity sensing properties through conductivity and curvature measurements. These smart composite films, capable of responding to humidity gradients, hold significant promise for developing actuators for non-contact human-machine interfaces, energy harvesting, and advancing soft robotics.

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3.Tzoumani, I.; Druvari, D.; Andrikopoulos, A.C.; Dominguez-Alfaro, A.; Malliaras, G.G.; Kallitsis, J.K. Facile Fabrication of Dual-conductivity, Humidity-responsive Single-layer Membranes: Towards Advanced Applications in Sensing, Actuation, and Energy generation. *J. Mater. Chem. C*, **2024**.

Preparation of Nanocomposite Fe_2O_3/TiO_2 Film Electrodes for the Development of a Voltammetric Sensor for Paracetamol

E. Topoglidis[1], E. A. Economou[1], C. S. Leva[1], P. Nikolaou[1], I. Koutselas[1],
[1]*Department of Materials Science, University of Patras, Rio 26 504, Greece*

Abstract: Nanocomposite electrodes of hematite (α-Fe_2O_3) deposited on mesoporous TiO_2 films on an indium tin oxide (ITO) glass substrate were found to serve for the development of a simple, relatively low cost, sensitive, voltammetric paracetamol (PAR) sensor. These modified TiO_2 films seem to exhibit improved conductivity compared to bare TiO_2 films, using an organic solvent, in particular dichloromethane (DCM). TiO_2 shows no electrochemical sensing towards paracetamol, while here α-Fe_2O_3 is doping effectively the TiO_2 due to its lower energy band gap, while the organic solvent assists, among other reasons, to avoid water splitting effects at the otherwise catalytic α-Fe_2O_3 surface. In addition, PAR seems to dissolve much better in DCM compared with an aqueous buffer. The electrodes' excellent electrochemical behaviour was examined by cyclic voltammetry as well as differential pulse voltammetry, while their structure was investigated by scanning electron microscopy (SEM), energy dispersive spectroscopy, Brunauer-Emmet- Teller analysis and X-ray diffraction. Under optimized conditions these electrodes exhibited excellent electrocatalytic behaviour towards PAR oxidation in the linear response concentration range from 0.1 to 20 μM (correlation coefficient 0.998) with a 0.080 μM detection limit. These sensors demonstrated good repeatability, reproducibility and stability, applicable for pharmaceutical PAR determination.

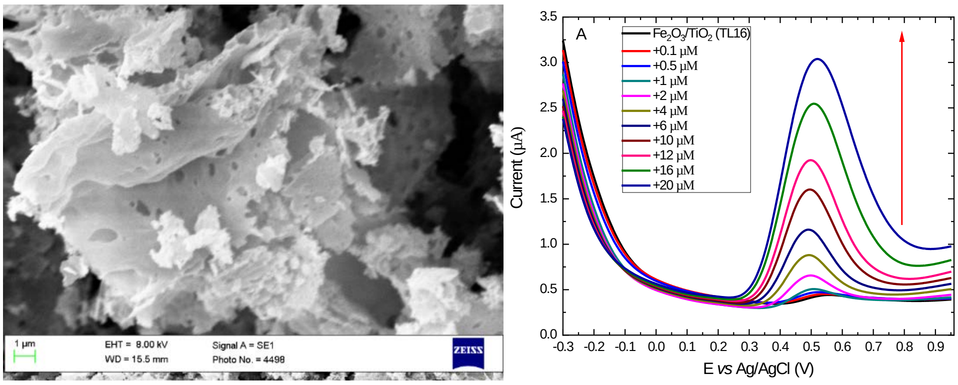


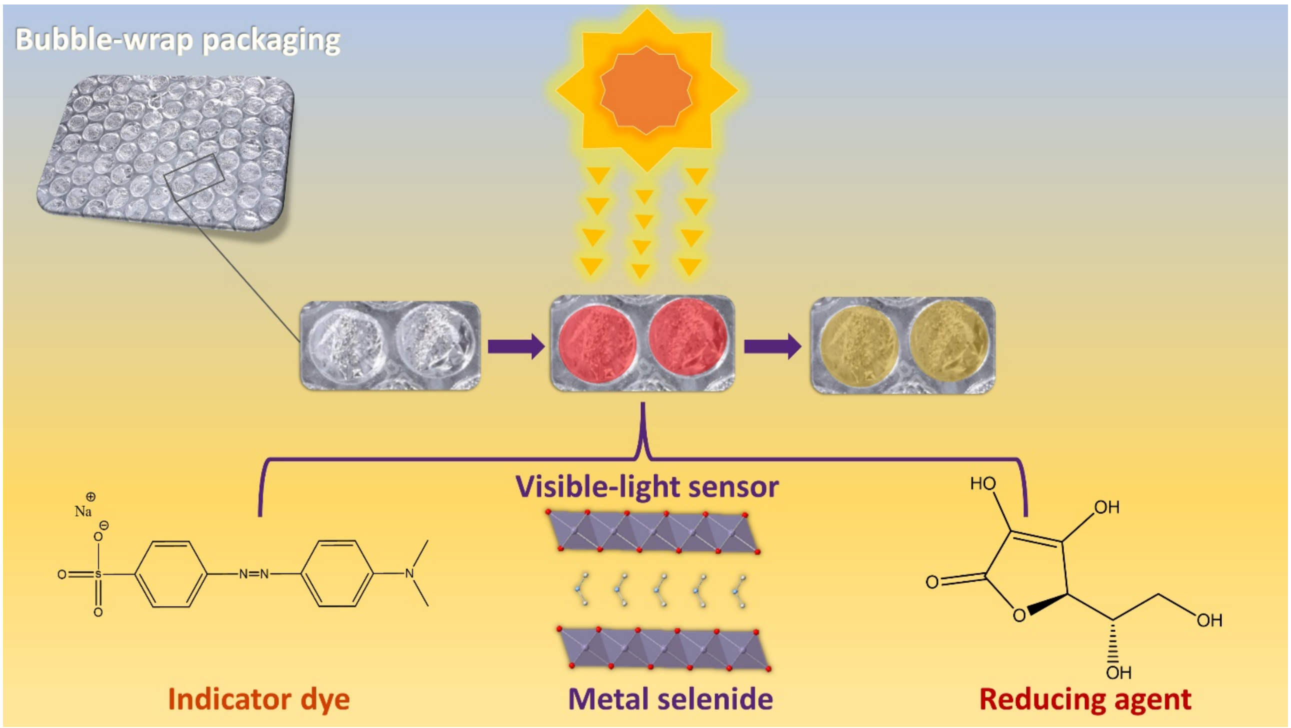
Figure: SEM image at 15kV of a Fe_2O_3-TiO_2/ITO film electrode (left) and Differential Pulse Voltammetry of a Fe_2O_3-TiO_2/ITO film electrode upon increasing concentrations of PAR in DCM-TBAH (right).

Funding: This research was partially supported by Grant 80669 from the Research Committee of the University of Patras via the "C. CARATHEODORI" program.

Monitoring exposure to sunlight using a new layered metal selenide visible-light photocatalyst incorporated in bubble wraps packaging material

Vasiliki I. Karagianni, Andronikos Georgiadis, Christos Lykos, Athanasios G. Vlessidis, Ioannis Konstantinou, Manolis J. Manos and Dimosthenis L. Giokas
Department of Chemistry, University of Ioannina, 45110, Ioannina, Greece

Abstract: This work demonstrates that a common packing material, “bubble wraps” (Aeroplast), can be utilized to serve as a probe to visible sunlight exposure. Hence, we have synthesized and thoroughly characterized a layered metal selenide photocatalyst with the general formula $(DMAH)_{2x}Mn_xSn_{3-x}Se_6$ **(DMSe-1)** (x= 1.3-1.7; $DMAH^+$=dimethylammonium), featuring a narrow band gap of 0.76 eV. Consequently, a photochemically sensitive probe based on this new catalyst, an indicator dye, and a reducing agent was prepared to assess exposure to visible light directly. The probe is added to air-filled bubble wrap compartments, undergoing photocatalytic degradation to provide a chromatic response to sunlight exposure. The probe's sensitivity to variable irradiation dose is customizable by adjusting the amount of the photocatalyst while the color intensity is related to the absorbed irradiation dose. The results from the new photoactive material strongly correlate with those from standard sunlight pyranometers (r = 0.98, p=0.05), demonstrating that bubble wraps, beyond their protective coating function, can effectively serve as a visible light sensor with an average error of <15%. Moreover, the study's findings encompass an advancement in using metal chalcogenides as visible light sensors, which could contribute to developing new light-sensitive materials.



Transparent conductive oxide (TCO) thin films as hydrogen gas sensors

E. Gagaoudakis[1], C.-P. Tsichlis[1], A. Sfakianou[1,2], V. Binas[1,2]
[1]Foundation of Research and Technology - Hellas, Institute of Electronic Structure & Laser (FORTH-IESL), Heraklion Greece
[2]Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece

Abstract: Hydrogen is known as the fuel of next generation. Thus, already the hydrogen industry affects the biggest global economies. However, hydrogen gas is an odourless, flammable and explosive gas, under specific conditions (4% in air). As a result an urgent need of hydrogen gas sensors, in order to monitor the hydrogen concentration during its production, storage, transportation as well as during its use. A great variety of materials have been investigated till now as gas sensing elements for hydrogen detection, such as metal oxide semiconductors, carbon based materials, 2-D materials and metal thiocyanates.

In this work, dc sputtered ZnO:Al films, grown at room temperatures, were tested against hydrogen gas of different concentrations, at elevated temperatures from Room Temperature (RT, 25°C) up to 400°C. Moreover, the films were characterized by X-Ray Diffraction (XRD) technique, Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), Energy Dispersive Spectroscopy as well as by UV/Vis/NIR spectroscopy, in order to determine their structural, morphological and surface properties, their stoichiometry as well as to their optical energy band gap.

In Fig. is presented the response of ZnO:Al thin films against different hydrogen gas concentrations, at 300°C. It can be seen that the ZnO:Al-based gas sensor has the ability to detect a low concentration of 100 ppm indicating that is a possible candidate material as hydrogen gas sensing element.

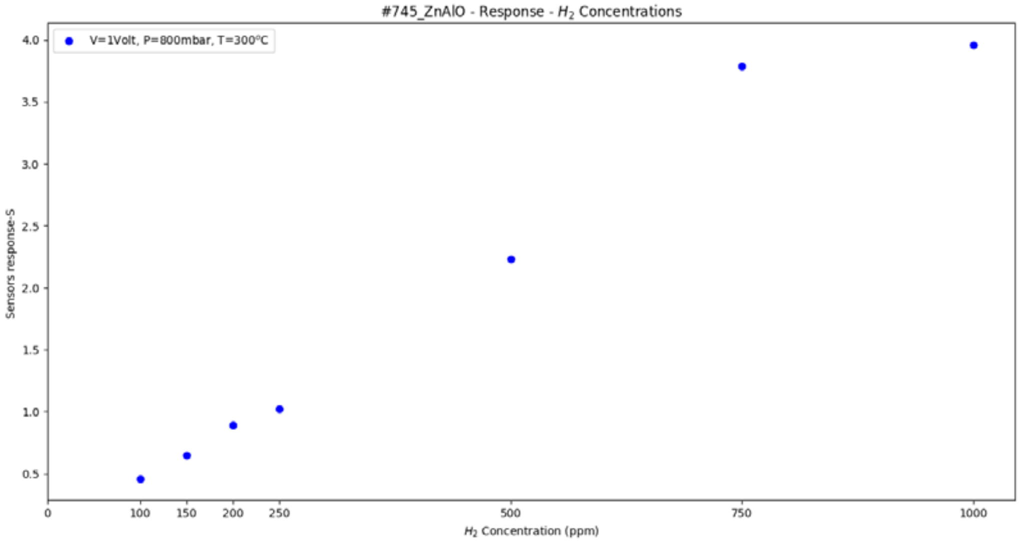


Figure 1: Response of ZnO:Al-based gas sensor against different hydrogen concentrations, at 300°C.

Acknowledgements

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Fabrication of new Co28Cr6MoxNb Alloy for Surgical Implants Using Vacuum Arc Remelting: Evaluation of Surface Degradation Response

S. Emmanouilidou[1], Z. Siaraka[1], I. Tzala[1], A. G. Lekatou[1]
[1]*Laboratory of Applied Metallurgy. Department of Materials Science and Engineering, School of Engineering, University of Ioannina, 451 10, Greece*

Abstract

This study aims to evaluate the impact of adding 0-3% Niobium (Nb) on the microstructure, mechanical properties, and resistance to corrosion and sliding wear of a CoCrMo biomedical alloy produced using Vacuum Arc Melting (VAM). The primary objectives are: a) to assess the suitability of VAM for fabricating biomedical CoCrMo in terms of surface degradation, and b) to evaluate the corrosion and wear resistance of Co28Cr6MoxNb alloys (x=0-3% Nb).

For the evaluative approach, the prepared samples were remelted five times in a VAM furnace to ensure a uniform microstructure. The microstructure was examined using X-Ray Diffraction, Optical Microscopy, and Scanning Electron Microscopy (SEM/EDX). Corrosion resistance was tested through cyclic potentiodynamic polarization in simulated body fluid (SBF) at 37°C and pH 7.4. The dry sliding wear behavior was analyzed using the ball-on-disk technique.

The main findings revealed that the Co28Cr6MoxNb VAM specimens exhibited a finer microstructure and greater microhardness compared to the Nb-free VAM-prepared counterparts. Additionally, the Co28Cr6MoxNb alloy demonstrated very high resistance to both general corrosion and localized corrosion, and true passivity in SBF solution at 37°C. Very low wear rates were also observed. Overall, the Co28Cr6MoxNb alloy showed superior surface degradation resistance compared to both the Nb-free VAM-prepared counterparts and commercial CoCrMo alloys fabricated by Selective Laser Melting (SLM).

Ubiquitous Carbons – A material for all occasions

S. Ravi P. Silva
Advanced Technology Institute, University of Surrey, Guildford, GU2 7XH, UK

Abstract:

Carbon as a material is unique. It can be observed with many phases and structures. This allows for a truly versatile and specialist building block which can be designed and synthesised to create designer materials to suite bespoke applications. The bonding hybridisation between carbon atoms, arising from their low affinity towards gaining or losing electrons allows for the well-known allotropes of diamond and graphite, and more recently discovered fullerenes, nanotubes and graphene. It facilitates for the building of platforms which links organics to inorganics and thereby extending to many other systems that can serve as platform technologies. The secret of building such technologies is the ability to create bespoke designer materials created at the nanoscale that can facilitate a structure for all occasions. Over the past few decades there have been a number of new applications and technology platforms introduced as a result of the better understanding of the element carbon and its properties. The structure, topology, chemical, mechanical and opto-electronic properties, all are dependent on the bonding hybridisation in carbons. In this talk we will build on the many decades of research conducted on carbon-based materials starting with the use of inorganic thin diamond-like carbon layers to dimensionally stable “space skins” on future space structures including for satellites. The ability for carbon bonds to hybridize between sp2 and sp3 character helps create specific modalities suitable for unique functionality. C60 and CNT based structures, allows for the versatility of the sp2 hybridized carbons to be optimised for optoelectronic applications. Highly defined CNT structures with known opto-electronic properties have given rise to Vantablack and facilitates a perfect test-bed for nanoelectronic devices. The ability to produce CNT at low temperatures allows for a plethora of new device applications to be coupled to designer chirality materials for next generation electronic systems.

Layered III-VI monochalcogenides for broadband optoelectronics

Kalyan Jyoti Sarkar. Zdenek Sofer
Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic

Abstract:

A large number of promising two-dimensional (2D) semiconductor materials, represented by black phosphorus (0.3 eV), transition metal dichalcogenide (TMDCs) (<2 eV), and hexagonal boron nitride (6 eV), have been extensively studied in optoelectronic devices. However, the spectrum of large-band gap materials remains very narrow, limiting the application for broadband optoelectronic devices. The broad family of III–VI monochalcogenides are a relatively unexplored part of the layered semiconductor family with the intralayer structure X–M–M–X, where M is a group III element (Ga, In) and X is a chalcogen (S, Se, Te). We present the synthesis and fabrication of high-performance broadband photodetector based on a few layers of GaTe with different dopants (Zn, Cd, Sb). The polarity of dopants was characterized by Hall measurements. Also, we have fabricated heterojunctions with few layers Zn-doped GaTe (p-type) and As-doped GaSe (n-type). Fabricated devices were irradiated with different wavelengths (300-1100 nm) of light, showing outstanding responsivity with low dark current and a high on/off ratio. Time-resolved photocurrent measurements were also performed, which exhibit a fast response time. We have calculated the electronic band structure and density of states of the samples. We also have designed photodetectors using multiscale modeling to explore the device's performance. By using a semiconductor module for theoretically modeled devices, the terminal current across the device with respective wavelength was calculated and compared with the experimental results.

Towards the Fabrication of Biocompatible Titanium Nitride Nanoparticles for Optical Hyperthermia Applications

T. Odutola[1], N. Pliatsikas[1], S. Panos[1], I. Tsamesidis[2], S. Kassavetis[1], E. Kontonasaki[2], J. Arvanitidis[1], D. Christofilos[3], M. Tzitiridou[4], M. Gioti[1], P. Patsalas[1]

[1]Department of Physics, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece
[2]School of Dentistry, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece
[3]School of Chemical Engineering and Physics Laboratory, Faculty of Engineering, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece
[4]Department of Midwifery, University of Western Macedonia, GR-50200 Ptolemaida, Greece

Abstract: Titanium Nitride NPs are a really promising plasmonic material for biomedicine. In contrast to the traditional plasmonic materials, such as Au, Ag and Cu, TiN is refractory and has a higher melting point. Furthermore, by doping and adjusting the Ti & N percentages, one could easily tune its spectrum and its localized surface plasmon resonance (LSPR) peaks, according to the desired application. These materials present LSPR peaks in between the biological window. Thus, they can be used as biomedical carriers for optical hyperthermia. In this work, we used pulsed laser ablation in liquids (PLAL) method to irradiate targets that were synthesized by reactive magnetron sputtering (RMS). RMS is a method that provides pure polycrystalline samples with well-controlled quantities and no oxidation. We had NPs produced in water by laser ablation in different wavelengths (355nm, 532nm & 1064nm), using the same laser power. We performed hemolysis and MTT assays to receive a preliminary estimation of their biocompatibility. Furthermore, we wanted to understand how the different laser wavelengths influence the samples' cytotoxicity. Both the hemolysis and the MTT assays showed promising results, as the cells' hemolysis was under 2,5% and the vitality was 70% or more, a fact really important because our material is raw, without any shell biofunctionalization, with the possibility of further improvement. The nanoparticles were also tested regarding their photothermal performance, displaying high photothermal efficiency. Concluding we synthesized efficient nanoparticles that could be a promising precursor for biomedical applications, such as optical hyperthermia.

Polarisation-encoded BB84 QKD for fiber and wireless channels

Giannis Giannoulis[1], Argiris Ntanos[1], Aristeidis Stathis[1], Dimitris Zavitsanos[1],
Nikolaos Lyras[1], Hercules Avramopoulos[1]
[1]School of Electrical and Computer Engineering, National Technical University of Athens,
9 Iroon Polytechniou Street, Zografou, Athens, 15772, Greece

Abstract: Following the original proposal of BB84 protocol [1], the polarization-encoded photons are naturally chosen as the information carrier in the Quantum Key Distribution (QKD) system. Polarization encoding of weak coherent pulses is common for free-space applications, since the atmosphere, unlike telecommunication optical fibers, keeps the polarization stable. Leveraging the mutually conjugated basis states of polarized single photons, deployable QKD systems can be prototyped in laboratory. In this presentation, polarisation modulation based on a Sagnac interferometer [2], polarisation state tomography based on polarisation handling elements (polarisation beam splitters, waveplates) and countermeasure strategies against polarisation drifts are briefly introduced, focusing on the challenges and the potential of implementing polarisation-encoded QKD systems for fiber, free-space and satellite quantum transmission links. Recent results from Photonics Communications Research Laboratory (PCRL) QKD transmission experiments are also presented (Fig1(a)).

Aside from the bulky, fiber-based implementations, Prepare-and-Measure (P&M) QKD protocols, BB84 QKD transmitter chip demonstrations have been presented using integrated photonics, showing high secret key generation rates and robust operation in free-space channels for polarisation-encoded qubits. In this context, we propose a novel polarization encoder system based on a Mach-Zehnder Interferometer, suitable for chip-scale implementation using Photonic Integrated Circuits (PICs). Leveraging the Jones calculus, the Stokes vectors of the obtained states can be calculated for the targeted states. The QKD performance metrics of the chip under realistic imperfections are then calculated using the Stokes formalism (Fig. 1(b)) and they were validated using alternative methods based on Poincare sphere representation. Our proposed MZI-based polarization encoding scheme demonstrates low intrinsic Quantum Bit-Error-Rate (iQBER) values.

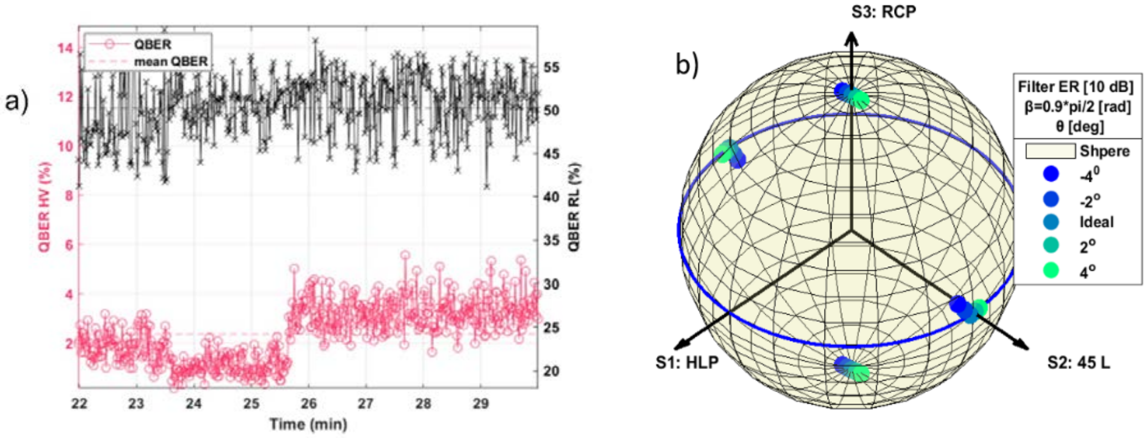

Fig.1. a) QBER values measured in Z-basis and Y-basis with and without coexistence over a 2.2km deployed fiber link. b) Poincare sphere representation of polarisation states for non-ideal performance of components.

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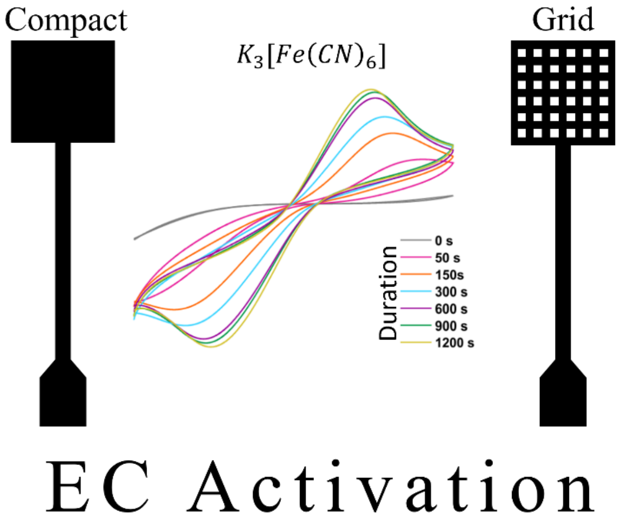
Electrochemical activation of carbon black – polylactic acid (CB/PLA) 3D printed electrodes for advanced electrochemical applications

A. Papavasileiou[1], L. Děkanovský[1], L. Chacko[1], B. Wu[1], J. Luxa[1], J. Regner[1], J. Paštika[1], Z. Sofer[1]

[1.] *Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 16628 Prague 6, Czech Republic*

Abstract:

Commercial conductive filaments are not optimized for electrochemical applications, leading to 3D-printed electrodes with limited exposed conductive surfaces and poor electrochemical performance, thereby hindering their use in energy and sensing technologies. Selecting an appropriate activation method is essential to unlock their full potential for their implementation in advanced applications. In this work, we propose electrochemical activation as a sustainable, time-efficient, and highly reproducible method to enhance the electrochemical performance of 3D-printed electrodes fabricated from Carbon Black–Polylactic Acid (CB/PLA). The layout of the electrode (compact and grid) (Scheme 1), and the activation duration are meticulously analysed to gain deeper insights into their impact on electrochemical behaviour. The CB/PLA 3D-printed electrodes are characterized electrochemically, structurally, and morphologically, and evaluated as platforms for i) electrocatalytic water splitting, ii) Zn-ion batteries, and iii) electrochemical sensors.



Scheme 1. Graphical illustration of compact and grid layout of the CB/PLA 3D printed electrodes and the influence of EC activation duration in the electrochemical behaviour of the electrodes.

Dielectric properties of Natural Ester Oil-Based Nanofluids with Iron Oxide Nanoparticles

Thomas E. Tsovilis[1], Evangelos T. Staikos[1], Alexandros Y. Hadjicostas[1],
Zacharias G. Datsios[1], George Litsardakis[2], Eleftheria C. Pyrgioti[3], George D. Peppas[4]

[1]High Voltage Laboratory, School of Electrical & Computer Engineering,
Aristotle University of Thessaloniki, Greece
[2]Laboratory of Materials for Electrotechnics, School of Electrical & Computer Engineering,
Aristotle University of Thessaloniki, Greece
[3]High Voltage Laboratory, Electrical & Computer Engineering Department,
University of Patras, Greece
[4]Research & Development Department, Raycap SA, Industrial Area of Drama, Greece
now at School of Electrical & Computer Engineering,
Technical University of Crete, Chania, Greece

Abstract: Oil-based nanofluids are a promising alternative to mineral oils that are traditionally utilized as insulating fluids in power industry applications such as power transformers. Besides being more environmentally friendly, natural ester oil - based nanofluids incorporating oxide nanoparticles have been found to enhance the dielectric strength and thermal conductivity of the liquid matrix. Materials characterization and composition optimization, theoretical interpretation of the nanofluid performance, as well as issues of long-term stability re subjects of the research in field.

In this work the effect of the concentration of iron oxide nanoparticles on the complex relative permittivity and on AC and DC conductivity of the natural ester oil nanofluid, for concentrations of 0.005% w/w, 0.05% w/w, and 0.5% w/w are examined, in the frequency range of 50 Hz – 1 MHz, at 167 V/m or at voltage levels of 0.5, 2 and 200 V, by means of an Impedance Analyzer (Keysight E4990A-120), an LCR meter (Hioki 3532-50) and a variable-frequency power supply, in combination with the Keysight 16452A and WTW MPA 12T liquid fixtures.

The real part of relative permittivity increases up to ~2% with nanoparticles concentration, a trend that has been observed for the low-frequency range at higher electric fields as well. The imaginary part of relative permittivity increases up to ~7 times with nanoparticles concentration, resulting in significant increase of the AC conductivity of the nanofluids at higher concentrations, where agglomeration occurs, remaining nevertheless lower than 10^{-12} S/cm for frequencies lower than 400 Hz. DC conductivity increases with applied voltage and concentration, being lower than AC conductivity, as expected, while it is noteworthy that the time duration of electrification (up to 1 min) did not exert any influence on the DC conductivity. The results are further discussed, and a study of dynamic breakdown voltage characteristics is underway.

Polypropylene based Hydromagnesite-Huntite and Magnesium dihydroxide flame retardant compounds

E. Mitropoulou[1,2], A. Soto Beobide[1], G. Mathioudakis[1], P. Tsaousis[1,2], K. Papapetros[1], K.S. Andrikopoulos[1,3] G. Voyiatzis[1]

[1] Foundation for Research & Technology-Hellas (FORTH), Institute of Chemical Engineering Sciences (ICE-HT), Stadiou Str., Rio-Patras, GR-265 04, Greece
[2] Department of Chemistry, University of Patras, Patras, GR-265 04, Greece
[3] Department of Physics, University of Patras, Patras, GR-265 04, Greece

Abstract: Polypropylene (PP) is a thermoplastic polymer, widely used in various applications due to its attractive properties such as chemical resistance, elasticity, toughness etc. However, like most polymers, it is highly flammable. For this reason, enhancing its flame-retardant (FR) properties is crucial due to safety requirements. Meanwhile, the concerns regarding the use of toxic halogenated flame retardants continues to grow, leading to ongoing research for alternative solutions, such as mineral based and inorganic flame retardants.

In this context, PP based compounds containing mixtures of huntite and hydromagnesite, minerals commonly found in Greece and Turkey, were prepared. The endothermal decomposition of these minerals happens on a wide temperature window with hydromagnesite's decomposition taking place between 220-400^{o}C, producing water, CO_2 and MgO char, while huntite's decomposition between 400-700^{o}C produces CO_2, MgO and CaO char. The vapors produced when the sample is enflamed dilute the oxygen necessary for combustion, while the char created on the polymer's surface insulates it, providing fire resistance. The most beneficial hydromagnesite-huntite ratio was proven to be a 3:1 mixture.

Similarly, magnesium hydroxide $Mg(OH)_2$ fillers, commercial and lab derived, were also used in PP based compounds. $Mg(OH)_2$ decomposes during an endotherm reaction that produces MgO and water. To improve its incorporation in the PP matrix, $Mg(OH)_2$ was surface modified. Functionalization with stearic acid or an organometallic titanium-containing surface modifier resulted in more uniform dispersion of $Mg(OH)_2$ in the PP matrix compared to raw $Mg(OH)_2$.

Samples produced with either huntite-hydromagnesite mixtures or $Mg(OH)_2$ showed enhanced fire retardancy at high filler loadings. The fire retardancy of the samples was assessed using an in-house LOI setup. The samples were also characterized using various analytical techniques, including FTIR/ATR, XRD, Raman, SEM and TGA providing insight on their physicochemical and structural properties.

*Acknowledgements: The results presented have received funding from the Eurostars 3 - Call 3 joint programme with co-funding from the European Union Horizon 2020 research and innovation programme (ID Number 2314, **F**lame **R**etardant **poly**mers **com**posites for advanced mattress development -FR.poly.com).*

In-situ One-Step Engineering of Hybrid CdS/TiO_2 Quantum Dots via Flame Spray Pyrolysis

C. Dimitriou, Y. Deligiannakis*

Laboratory of Physical Chemistry of Materials & Environment, Department of Physics, University of Ioannina, 45100 Ioannina, Greece

**ideligia@uoi.gr*

Abstract: Quantum dots (QDs), which are quasi-zero-dimensional semiconductor nanomaterials, has garnered substantial scientific interest.[1] These nanostructures confine excitons in all three spatial dimensions, leading to quantum confinement effects. As a result, their energy levels become quantized into discrete states, distinguishing their optical and electronic behaviors from those of larger-scale materials.[2] Hereunder, we have produced CdS/TiO_2 quantum dot hybrids through Flame Spray Pyrolysis (FSP) process,[3,4] where – in addition to CdS QDs – the TiO_2 matrix was also QD-size (3 nm).

The CdS/TiO_2 QDs were synthesized using a novel FSP reactor-design equipped with an open spray injection system (SI-FSP). Using this technology, we have produced a library of CdS/TiO_2 hybrids where 3 nm CdS QDs were deposited on either 20 nm TiO_2 or 3 nm TiO_2-QD. By controlling FSP parameters, the TiO_2 particles were formed within the flame, followed by an *in-flight* deposition of CdS on the TiO_2. X-ray diffraction (XRD) analysis confirmed diffraction peaks corresponding to both CdS, with particle sizes of 3 nm and TiO_2 with particle sizes 3 or 20 nm, respectively. Using Raman, XPS and UV-Vis spectroscopies, we studied the physics of the CdS/TiO_2 QDs interface. The data show that interfacial S-Ti states are formed, as well as Ti^{3+} states, indicating electrons transfer from the S to the Ti-lattice, in the dark. The photogeneration of {hole-electron} Wannier-type pairs by photoexcited CdS/TiO_2 was studied using *in-situ-irradiation* Electron Paramagnetic Resonance (EPR) spectroscopy. All these data provide evidence that the novel one-step FSP engineering is a potent technology for scalable-production of complex nano-assemblies via control of nanolattice at the Quantum-Size limits at the same time preservice the key functionalities of the nanocrystals.

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Effect of Quantum Dots on Nematic Phases of Mesogenic Dimers

S. B. Atata, I. Lelidis
Faculty of Physics, National and Kapodistrian University of Athens, Panepistimiopolis, Zografos, 15784 Athens, Greece

The twist-bend nematic phase (N_{TB}) is a unique liquid crystal (LC) mesophase, where achiral bend-shaped molecules spontaneously form a locally chiral heliconical structure. Since its experimental discovery a decade ago, a great number of LCs and LC-LC compounds that exhibit a N_{TB} phase have been synthesized and investigated. However, research on the influence of nanoparticles on the N_{TB} structure as well as on its properties is still in its early stage.

We experimentally investigated the effect of surface-activated core-shell quantum dots (CdSe/ZnS) on both the uniaxial nematic (N) and N_{TB} phases of the liquid crystal 1″,9″-bis(4-cyanobiphenyl-4'-yl)nonane (CB9CB) using polarized optical microscopy (POM), birefringence, and electro-optical measurements. We explored the thermodynamic stability of nanocomposites resulting from quantum dots dispersion in the liquid crystal compound. We constructed the phase diagram of the nanocomposite systems as a function of temperature (T) and mass fraction (χ) of the nanoparticles. We studied the microstructure of the nanocomposites and measured their birefringence as a function of T and χ. In addition, using an electric field, we induced the reorientation transition in LC-cells of planar geometry. We measured the voltage threshold and switching times of the transition, as functions of T and χ. Finally, we also explored the impact of nanoparticle geometry on the reorientation transition and properties of the nanocomposites.

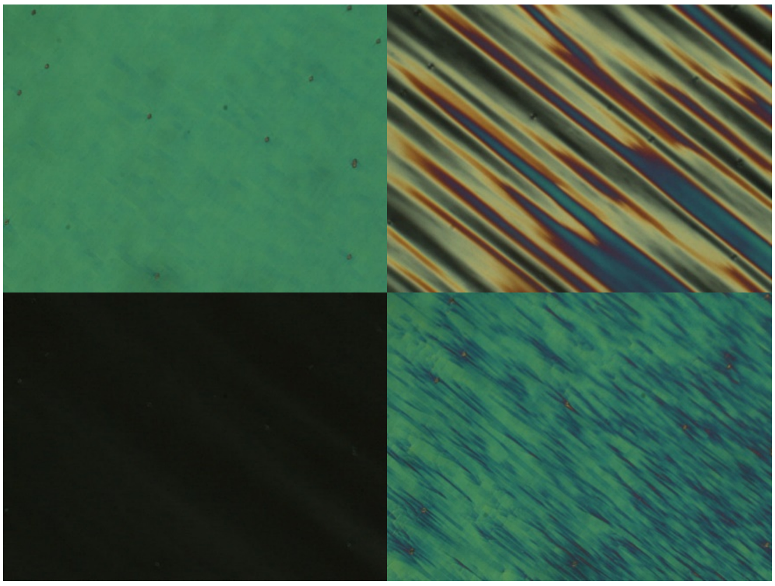

Figure 1. POM images of CB9CB in the twist-bend nematic phase. (a) Before the application of an electric field (E=0), (b) under the effect of the field (E ≠ 0), (c) when the director is parallel to the field (E ≠ 0), (d) when the field is turned off (E=0).

Topology Sorting: Separating Polymer Blend Components of Different Architecture by Infiltration in Nanochannels

P. Kardasis,[1] I. Tzourtzouklis,[1] and George Floudas[1,2,3]

[1] Department of Physics, University of Ioannina, 45110 Ioannina, Greece
[2] University Research Center of Ioannina (URCI) - Institute of Materials Science and Computing, 45110 Ioannina, Greece
[3] Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Abstract: We report the imbibition and adsorption kinetics of a series of symmetric linear/star cis-1,4-polyisoprene blends within the long channels of self-ordered nanoporous anodic aluminum oxide (abbreviated: AAO). [1] Using *in situ* nanodielectric spectroscopy,[2] we followed the evolution of the longest chain modes in the blends with a judicious selection of molar masses for the components. We demonstrated differences in the imbibition kinetics of linear and star components based on the relative viscosities (*e.g.*, polymers with lower zero-shear viscosity penetrated first the nanopores). [3,4,5] Following the complete imbibition of the pores, the adsorption time, τ_{ads}, of each component was evaluated from the reduction in the dielectric strength of the respective chain modes. In the majority of blends, both components exhibited slower adsorption kinetics with respect to the homopolymers. The only exception was the case of entangled stars mixed with shorter linear chains, the latter acting as a diluent for the star component. This gives rise to what is known as topology sorting, *e.g.*, the separation of linear/star blend components in the absence of solvent. Moreover, a simple relation ($\tau_{\mathrm{ads}} \sim 10 \times t_{\mathrm{peak}}$; t_{peak} is the time needed for the complete filling of pores) was found for linear polymers and stars. This suggested that the characteristic timescale of imbibition (t_{peak}) governs the adsorption process of polymers. It further implied the possibility of predicting the adsorption times of high molar mass polymers of various architectures by the shorter imbibition times.

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Time evolution of transitions between wetting states on slippery nanoparticle-based superhydrophobic surfaces.

C. Tsekeridis[1], D. Tzitzilis[1], I. Ntakoumis[1], P. Papadopoulos[1]
[1] Department of Physics, University of Ioannina, P.O. Box 1186, 45110, Greece

Abstract:

A major goal in coating research is the design of self-cleaning surfaces. The self-cleaning property results from trapped air pockets under the water droplets. Slippery Liquid-Infused Porous Surfaces (SLIPS) consist of two components: a porous solid substrate and a liquid stabilized on and within the substrate.

For most of the literature, it was taken for granted that the formation of the "fakir" Cassie-Wenzel state during droplet deposition implies that the air or lubricant layer is stable over time. Previous studies on porous superhydrophobic surfaces, show a slow penetration of liquids that has two negative effects: (a) the surface does not remain completely clean when droplets are removed, and (b) a part of the porous inorganic network breaks by moving the contact line due to capillary forces. The phenomenon is undesirable for many applications and has been attributed to a successive "depinning" of the contact line associated with thermal fluctuations.

In the present work we examine whether the phenomenon is observed in SLIPS. We show the construction of SLIPS based on silicon nanoparticles and study the penetration depth of various drops of low surface tension on these surfaces (alkanes, alcohols and PDMS). Experimentally, we used an optical tensiometer and a homemade laser scanning confocal microscope (LSCM). We have observed that the penetration rate decreases with time but is not as strongly dependent on the surface tension as on the superamphiphobic surfaces. To explain the phenomenon, we made numerical calculations using a system consisting of joined uniform spheres (nanoparticles) and minimizing Gibbs energy, examining the energy barrier. Additionally, we search the dependence of the energy barrier on pressure, the distance between the centres of the nanoparticles and the degree of sintering.

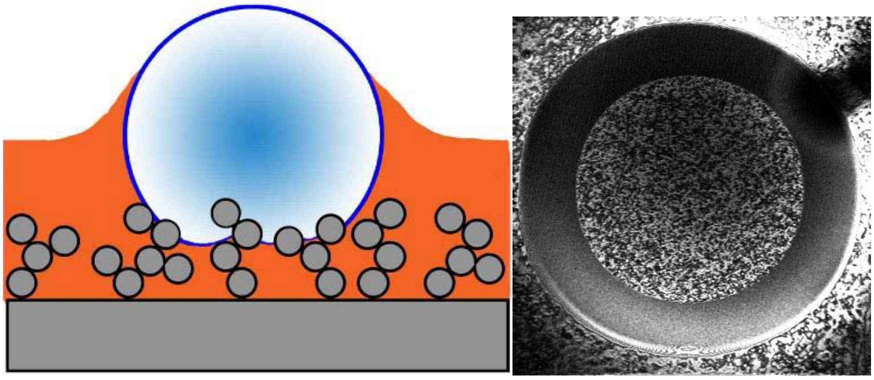

Figure 1: (Left): A water drop (blue) resting on a porous surface made of nanoparticles (gray) that is infused with a lubricant (orange). Schematic representation of a droplet on soot surface (grey) with lubricant (orange). (Right): Interference pattern generated by the flat surface of the cover slip, and the drop-lubricant and lubricant-air interfaces.

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Enhanced Ionic Conductivity in Innovative Single-Ion-Conducting Block Copolymer Electrolytes

M. Spyridakou[1], I. Tzourtzouklis[1], T. Gäb[2], H. Frey[2], G. Floudas[1,2,3]

[1] Department of Physics, University of Ioannina, P.O. Box 1186, 45110 Ioannina, Greece
[2] Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany
[3] University Research Center of Ioannina (URCI)-Institute of Materials Science and Computing, 45110 Ioannina, Greece

Single ion-conducting polymer electrolytes (SICPE) based polystyrene and poly(ethylene oxide) block copolymers (PS-*b*-PEO) show great potential, due to their durability and the ability to exclusive charge transport via lithium cations [1]. However, incorporating covalently attached anions into the flexible polyether block to yield SICPE is a synthetic challenge [1]. For this purpose, a new diblock copolymer electrolyte, polystyrene-*b*-poly(ethylene oxide-*co*-glycidyl methyl ether) (PS-*b*-P(EO-*co*-GME)), was synthesized bearing different [O]:[Li^+] ratios and different compositions [2]. The P(EO-*co*-GME) block can be engineered to simultaneously suppress the PEO crystallization and significantly enhance ion conduction. This reflects the lower glass temperature of PGME as compared to PEO, its inability to crystallize due to branching and the presence of two oxygens that can better solubilize lithium salts. In all investigated samples, X-rays scattering (SAXS) revealed strong nanophase segregation between the PS and P(EO-*co*-GME) blocks, while the ordered morphology is maintained, even at higher temperatures. The thermodynamic properties (DSC) verified the vitrification of the two blocks, identifying two glass temperatures and further confirming the absence of PEO crystallization. Ionic conductivity measurements performed as a function of temperature revealed enhanced conductivity values, in comparison to previous studies in the related PS-*b*-P(EO-*co*- LiTFSAEGE) [3], due to the considerably high conduction of the PGME. Simultaneously, the mechanical stability of the system is maintained by the glass PS block. This provides a promising alternative for designing SPEs, which combine high ion conductivity with mechanical stability, both of which are important for future battery technologies.

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Wrinkling of thin laser annealed films

M. Emerse[1], L. Goehring[1], N. Kalfagiannis[2], D. Koutsogeorgis[1]
[1]School of Science and Technology, Nottingham Trent University, Nottingham NG11 8NS, United Kingdom
[2]Department of Materials Science and Engineering, University of Ioannina, Ioannina 45110, Greece

Abstract: Thin films will often spontaneously wrinkle when they have a differential strain, with respect to their substrate. Such wrinkling instabilities can explain phenomena like the crinkling of leaves and flowers, and the folding of the brain, for example. Similarly, control over wrinkling patterns is used to template surfaces with bespoke frictional, tactile, or optical properties, and to accommodate excess strain in flexible electronics.

We report on the use of laser annealing to induce controlled wrinkle patterns. Thin silica films, between 10-200 nm, are grown on silicon wafers by thermal oxidation in an ambient atmosphere. These films are then exposed to a brief, intense laser pulse, at a wavelength of 248 nm, with a 25 ns pulse duration and fluence of 250-1500 mJ/cm^2. At this wavelength, the silica is effectively transparent, and the laser energy is preferentially deposited into the near-surface silicon. Both the silicon and silica heat up as a result, and then rapidly cool back to room temperature. The thermal expansivity of silicon is much larger than that of silica, and so the silicon substrate expands and contracts much more significantly than the superficial silica film.

At lower fluences, the silica/silicon interface heats up, but cools again without any significant permanent deformation: the treatment is reversable. However, above well-defined threshold conditions, corresponding to the melting of the interfacial silicon, wrinkles remain after laser annealing. We argue that the interfacial melting resets the interfacial stress at elevated temperatures. Cooling back down then introduces a misfit strain, placing the silica into effective compression as the silicon contracts. These conditions drive surface wrinkling (see Figure), with a wavelength and amplitude that depend on the silica film thickness, and the depth of the melted layer.

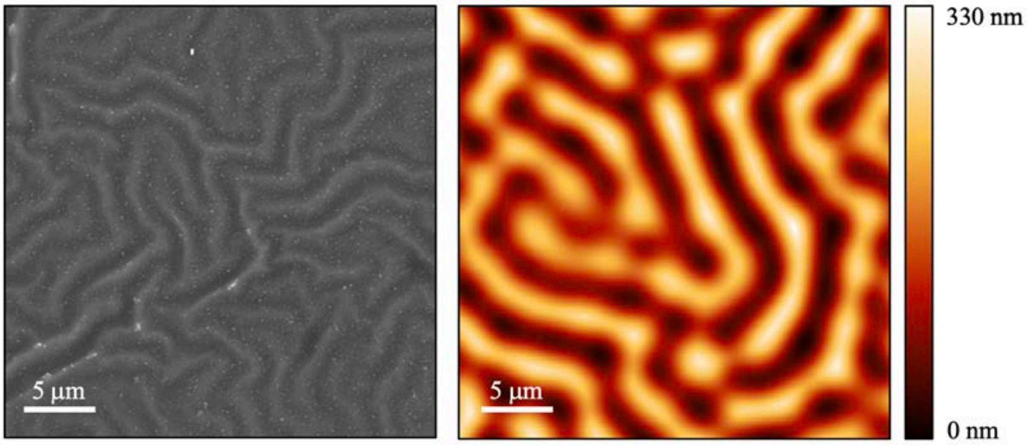

Figure 1: SEM (left) and AFM (right) of wrinkles in laser annealed films.

Laser-assisted transformation of electrospun PAN fibers into graphene: Insights from surface chemistry studies and spectroscopy

Amirali E.[1], Chronopoulos I.[1], N. Samartzis[1], Yannopoulos S.N.[1,2], Sygellou L.[1 *]

[1] Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE-HT), Patras, 26504, Greece

[2] Physical Chemistry Laboratory, Department of Chemistry, University of Patras, Rio-Patras, 26504, Greece

Abstract: Polyacrylonitrile (PAN) is a rigid thermoplastic material widely used in carbon fiber production, textile manufacturing, and water and air filtration due to its versatility, which depends on its chemical modification through stabilization and graphitization processes. Oxidative stabilization of PAN not only prevents fiber melting but also reduces carbon volatilization during subsequent carbonization. Stabilization involves controlled annealing at temperatures between 200 and 300 °C, transforming the polymer backbone from linear to lateral, forming an aromatic ladder structure that enhances thermal stability for graphitization. This step entails breaking C≡N bonds and forming C=N (pyridinic) and C–N (pyrrolic) bonds. In our study, an 8% wt. PAN solution was electrospun to produce fibers with 150-200 nm average diameter, subsequently stabilized at 280 °C in air for two hours. The sample was then irradiated with a CO_2 laser under ambient conditions, transforming it into porous graphene structures. The study aims to elucidate the structural evolution of PAN through (a) heat-induced stabilization and (b) laser-assisted graphitization to achieve high-quality, highly conductive graphene. Techniques such as X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and Raman spectroscopy were employed. XPS analysis provided insights into surface chemical modifications (C, O, N) including atomic ratios, carbon hybridization, and the transformation of carbon-nitrogen bonding into carbon sp^2 configurations, elucidating mechanisms of chemical change during each transformation step. SEM images revealed fiber morphology changes, while Raman scattering confirmed the high-quality graphene-like structure of the laser-assisted graphitized product. The high sp^2 carbon content and the retention of a distorted fiber morphology in the irradiated product account for exceptionally low sheet resistance of the graphene-like material, rendering it suitable for energy storage applications, such as in supercapacitors.

Titanium and Gallium Nitride Nanoparticles by Nanosecond Laser Ablation for Flexible Electronic

S. Panos[1], N. Pliatsikas[1], T. Odutola[1], S. Kassavetis[1], C. Papouli[1], J. Arvanitidis[1], D. Christofilos[2], M. Gioti[1], E. Pavlidou[1], P. Patsalas[1]

1 Department of Physics, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece

2 School of Chemical Engineering and Physics Laboratory, Faculty of Engineering, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece

Abstract: Nitrides are a leading material family for innovative nanotechnology applications and have revolutionized the semiconductors and consumer electronics industry. They are classified into two main categories: i) III-nitride wide-gap semiconductors (such as GaN and AlN) and ii) Conducting nitrides of IIIb-Vb transition metals (such as TiN, ZrN), which have recently gained importance as alternative plasmonic materials. While thin-film fabrication of nitrides is well-established and controlled, creating high-quality nitride nanoparticles (NPs) and developing nitride inks for flexible electronics applications remains open challenge. In our work, we propose an eco-friendly, proof of concept approach for nanomaterials with tailored properties using Pulsed Laser Ablation in Liquids (PLAL). We fabricated colloidal NPs by laser ablating films in liquids from both aforementioned categories of Nitrides, namely Titanium Nitride (TiN) and Gallium Nitride (GaN), employing a nanosecond Nd:YAG pulsed laser. TiN was studied at 3 different laser beam energies; energy of 5 mJ resulted in NPs mean size of 42 nm while smaller energy beam (1 mJ) produced NPs of 25 nm in size. Laser wavelengths of 355, 532, and 1064 nm did not affect the mean diameter of NPs, but noteworthy it influenced the crystalline quality. Specifically, shorter wavelengths resulted in TiN NPs with fewer defects, as evidenced by Raman analysis. Different solvents had also an impact in the colloidal TiN NPs providing oxidized NPs for aqueous solutions and a carbide coated NPs for organic solvent like acetone. For GaN, laser energy was studied for specific laser wavelength and liquid. We provide valid instrumentation for producing Quantum dots from GaN for optoelectronic applications. Preliminary results are shown, proving the concept of nanosecond laser ablation for this purpose.

Gradient Interatomic Potentials / GIP

K. Parisis[1], A. Konstantinidis[1], K.E. Aifantis[2], E.C. Aifantis[1,3]
[1]*Aristotle University of Thessaloniki, Thessaloniki, GR 54124, Greece*
[2]*University of Florida, Gainesville, FL 32611, USA*
[3]*Michigan Technological University, Houghton, MI 49931, USA*

Abstract: London was the first to rigorously derive his interatomic potential based on quantum mechanics principles. It featured an “attractive” $-1/r^6$ branch, which was cut off at an equilibrium distance r_0 where a repulsive force sets in. Lennard-Jones introduced in an ad hoc manner a “repulsive” $1/r^{12}$ branch and his resulting empirical potential is routinely used in a plethora of atomistic, molecular and discrete particle computer simulations for a variety of materials and processes. In the mid eighties – mid nineties the last author proposed a gradient modification of Hooke’s law of elasticity and von Mises flow rule of plasticity by introducing a Laplacian (∇^2) term and a corresponding internal length (IL) in the classical expressions. The resulting models of gradient elasticity and gradient plasticity became very popular until today since they can eliminate singularities, repair the mesh-size dependence of finite element calculations in the material softening regime, and interpret size effects in a robust manner. Recently, the (∇^2, IL) recipe was extended from the continuum (the so-called internal length gradient/ILG material mechanics framework [1,2]) to discrete level by using the London’s quantomechanical potential as an instructive example. This extension provides a “repulsive” branch in addition to the “attractive” one which results naturally from the solution of an inhomogeneous Helmholtz equation. By adjusting the IL parameter, it is shown that the so-obtained analytical expression for the gradient London potential can rigorously recover the empirical form of the Lennard-Jones potential. The idea of extending the ILG approach of the last author from the continuum to the discrete level was due to the third author, while the initial calculations were carried out by the first author and verified by the second one. The purpose of the presentation is to invite the solid state physics colleagues to consider the physical basis and viability of the ILG approach and utilize it to derive nonlocal gradient expressions for other types of potentials.

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3D bistable metamaterial mechanism based on auxetic rotating equilateral triangle structure

I.P. Dachis[1], E.P. Hadjigeorgiou[1]
[1]*Laboratory for Mathematical Modeling of Materials and Scientific Computing, Department of Materials Science and Engineering, University of Ioannina, GR-45110 Ioannina, Greece*

Abstract: Programmable matter, a captivating research field, explores materials with advanced properties. Bistable metamaterials are structures with tailored transformation characteristics. In our study, we created a bistable 3D metamaterial mechanism with shape programming capabilities. Notably, our 3D structure extends the 2D rotating equilateral triangle auxetic topology, resulting in both bistability and a negative Poisson’s ratio. Additionally, we employed a transformation function to analyse the material’s properties as a continuum body.

Synchronization of random walking oscillators

Konstantinos Tsachalinas[1], Chariton Polatoglou[2]
[1,2]*School of Physics, Aristotle University of Thessaloniki, Greece*

Abstract:

In the heart of this work are complex systems simulations, based on a stochastic model of interacting agents. Starting from the core principles of the NetLogo's "Fireflies" optical oscillator model (Wilensky, 1997), the new model "fireflies-rw" is modified by (a) the treatment of the oscillator-agents as classical random-walkers interacting on a square 2D lattice, and (b) the introduction of the oscillators' discrete phase order n. To support this model, a new simulation software has been developed, allowing the investigation of collective statistical properties in variable-density populations of oscillator-agents. This investigation covers the evolution of the systems from random initial conditions all the way to their complete self-organization (full oscillator synchronization), while tracking the emergence of notable collective behaviors exhibited by the complex systems.

Summarizing the key points of this research, we note the following: (1) In n-phase systems with agent density $0.5<d<1$ ($n=2, 10, 20, 30, 40$), the mean value of synchronization time, $\langle t_{sync}\rangle_n$, as a function of system density d, is well described by a power law. (2) There is bias in the distribution of terminating values of synchronization phase order n as a function of density d. (3) Moreover, dense multi-phase systems, throughout their evolutionary process from random initial conditions up to the point of global synchronization, are characterized by a sigmoid self-organization motif.

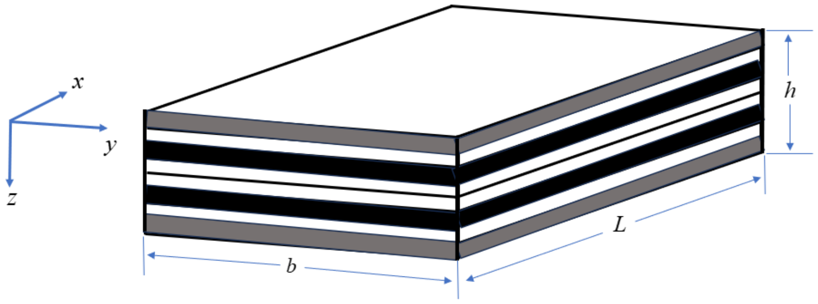
Modeling and analysis of laminated HSDT piezoelectric composite beams

K. I. Ntaflos[1], E. P. Hadjigeorgiou[1]
[1] *Laboratory of Mathematical Modelling of Materials and Scientific Computing,*
Department of Materials Science and Engineering, University of Ioannina,
University Campus 45110 Ioannina, Greece.

Abstract: Nowadays, multifunctional composite materials are used in a wide variety of applications and are preferred for the advanced mechanical, thermal, electrical and magnetic properties when compared to traditional materials. Plenty of research articles are available on the static deformation analysis of elastic laminated beams using refined shear deformation theories. Reddy gave analytical and numerical solutions to bending, buckling and free vibration problems of elastic laminated composite beams and plates. Nevertheless, further research is required in the field of the deformation of laminated elastic beams.

The present study deals with the modeling and analysis of piezoelectric laminated composite beams using higher order shear deformation theories (HSDT) and explores the effects of shear deformation on elastic and piezoelectric layers that often serve as substrate layers of multilayer composite sensors and actuators. Based on higher order shear elastic deformation and electric potential distribution theories, a general mathematical model is derived. Governing equations and the associated boundary conditions for a composite structure with n layers are developed using a generalized Hamilton's principle. The static behavior of the composite structure is investigated and various bending problems with different layers are solved.

Keywords: laminated composite structures; piezoelectric beams; multilayered piezoelectric sensors and actuators; higher-order shear deformation theories.



Rapidly-rotating quantum droplets confined in a harmonic potential

S. Nikolaou[1], G. M. Kavoulakis[1,2], M. Ögren[2,3]
[1]*Department of Mechanical Engineering, Hellenic Mediterranean University, 71004, Heraklion, Greece*
[2]*HMU Research Center, Institute of Emerging Technologies, 71004, Heraklion, Greece*
[3]*School of Science and Technology, Örebro University, 70182, Örebro, Sweden*

In recent years the problem of quantum droplets has attracted a lot of attention. Quantum droplets are self-bound states [1], which appear in binary mixtures of Bose-Einstein condensed atoms, when the beyond-mean-field (repulsive) energy term [2] balances out the mean-field (attractive) term. We investigated [3] a quantum droplet in two spatial dimensions, which rotates in a harmonic potential, focusing on the limit of “rapid” rotation, where the rotational frequency of the trap Ω approaches the trap frequency ω. We examine this problem mainly using a semi-analytic Wigner-Seitz approximation [4] for the description of the state with a vortex lattice, which forms in “large” rotating droplets. Working with a fixed rotational frequency Ω, as Ω approaches ω, we found that the mean spacing between the vortices decreases, while the “size” of each vortex increases as compared to the size of each cell, as shown in Fig. 1. In contrast to the well-known problem of contact interactions, where we have melting of the vortex lattice and highly-correlated many-body states, here no melting of the vortex lattice is present, even when $\Omega = \omega$. This difference is due to the fact that the droplet is self-bound. Actually, for $\Omega = \omega$, the “smoothed” density distribution becomes a flat top, very much like a static, unconfined droplet. When Ω exceeds ω, the droplet maintains its shape and escapes to infinity, via center-of-mass motion.

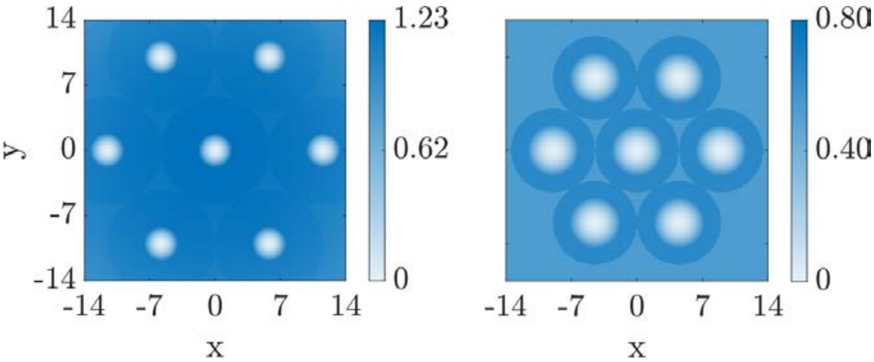


Figure 1: The density of the droplet around the origin for $\Omega < \omega$ (left), and $\Omega = \omega$ (right).

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THz graphene-based metasurfaces for wave manipulation

A. Tasolamprou[1],
[1]*National and Kapodistrian University of Athens, Department of Physics*

Abstract We discuss the unique possibilities stemming from exploiting the exotic properties of artificial metasurfaces designed for operation in the THz regime. Metasurfaces are electromagnetically ultrathin artificial materials with macroscopic properties defined by the architecture of the building blocks, the meta-atoms. Adjusting the meta-atoms enables the control over different aspects the electromagnetic waves and the realization of unusual electromagnetic functions. Within this framework we present groups of metasurface configurations incorporating different constituent materials. We mainly focus on graphene based metasurfaces acting as modulators for the THz regime. Graphene, the acclaimed two-dimensional (2D) material made of carbon atoms arranged in a honeycomb lattice, exhibits unique optical properties particularly in the THz spectrum, where it predominantly exhibits a Drude-like response. We focus on planar metasurfaces structures, starting from the simple metal-insulator-metal scheme to carbon nanotubes of variable number of interlayers and we show that the effective medium analysis unveils a rich palette of electromagnetic features that can be engineered by the adjustment of the geometry. Additionally we show that ultrafast modulation response can be assessed with the use of a broadband THz time-domain-spectroscopic system (THz-TDS) in an IR pump-THz probe configuration and also with nonlinear self-action. The proper design of the metasurface provides the means for achieving critical coupling and hence increased/perfect tunable absorption. The near-IR stimulus generates hot carriers in the graphene metasurface which effectively reduces its THz conductivity. Similar phenomenon can be induced by self-modulation using intense THz fields. The simple scheme of the absorber can be used as a platform for ultrafast flat optics and metasurfaces. Apart from that, we review additional recent THz metasurface findings with some interesting features.

Adjustable and Dynamic Metamaterials for Advanced Photonic Applications

N. Matthaiakakis[1], N. Dimogerontaki[1,2], S. Droulias[3], G. Kakarantzas[4], N. Kehagias[1]
[1] NCSR Demokritos, Institute of Nanoscience & Nanotechnology, P. Grigoriou 27 & Neapoleos Str., 15341 Ag. Paraskevi, Greece
[2] Department of Physics, School of Applied Mathematical and Physical Sciences National Technical University of Athens, Zografou Campus, GREECE
[3] Department of Digital Systems, University of Piraeus, Piraeus 18534, Greece
[4] Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 11635 Athens, Greece

Abstract: Metamaterials are transforming photonics by enabling precise control over light's properties, leading to novel applications across various fields. These engineered materials manipulate electromagnetic waves in ways that natural materials cannot, allowing for advanced linear and nonlinear optical operations. Initially, metamaterial properties were static, defined by their fabrication. Recently, significant efforts have focused on developing post-fabrication adjustable and dynamically tunable metamaterials[1]. Different mechanisms are under active investigation, including reconfigurable, liquid crystal, 2D material, phase-change, and nanoelectromechanical metamaterials.

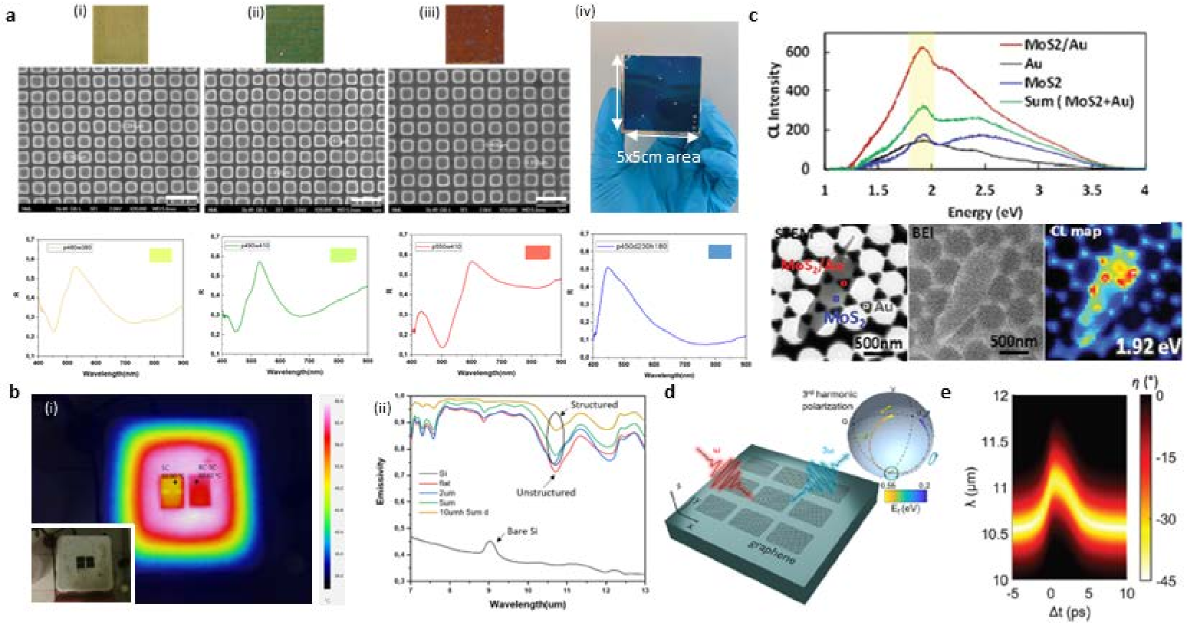

Figure 1. Adjustable and dynamically tuneable metasurfaces. a) Plasmonic colour pallet fabricated by nanoimprint lithography. Colours can be adjusted in post fabrication application of polymer resits with different refractive indexes b) Radiative cooling achieved through the formation of polymer-based metamaterials on arbitrary surfaces with the use of nanoimprint lithography. c) Metamaterial for emission enhancement of atomic film emitters (MoS_2)[3]. d) Electrostatically tuneable graphene-based metamaterial for the manipulation of the amplitude and ellipticity of the third harmonic [4]. e) All-optical ultrafast tuneable graphene metamaterial for high speed modulation of the ellipticity of reflected light[5].

Here, we present an overview of our contributions, highlighting our work on adjustable and ultrafast dynamically tunable metamaterials for linear and nonlinear optical processes. To realize adjustable metamaterials, we utilize nanoimprint lithography[2] and post-processing selective deposition methods (e.g., inkjet, laser ablation) of dielectric/metallic materials. For dynamically tunable metamaterials, we leverage the sensitivity of 2D material conductivity to external stimuli such as electric fields or high-intensity optical pulses.

By utilizing these methods, we demonstrate adjustable metamaterials in commercially significant fields such as plasmonic coloring (Fig. 1.a), radiative cooling (Fig. 1.b), and local emission enhancement (Fig. 1.c)[3]. Additionally, we showcase dynamically tunable metamaterials for controlling light's degrees of freedom on ultrafast timescales for both linear and nonlinear optical processes (Fig. 1.d,e)[4,5]. Finally, we explore the potential of roll-to-roll fabrication for upscaling and low-cost mass production. The presented advances pave the way for compact and multifunctional photonic devices with unprecedented versatility, offering transformative capabilities by controlling light flexibly and dynamically in a low cost, mass producible, and affordable manner.

Acknowledgements

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Extreme pulse shaping from saturable absorption in a critically-coupled graphene-loaded photonic crystal cavity

A. Dagkli[1], S. Doukas[1], A. Chatzilari[1], A.C. Ferrari[2], E. Lidorikis[1]

[1]Department of Materials Science & Engineering, University of Ioannina, Ioannina 45110, Greece
[2]Cambridge Graphene Centre, University of Cambridge, Cambridge CB3 0FA, UK

Saturable absorption in Single Layer Graphene (SLG) has played an important role in various applications, such as signal modulation, laser mode-locking, and others [1-6]. A critical quantity is the saturation intensity I_s, i.e., the incident intensity at which SLG absorbance drops to half its low intensity value. However, while critical, there are no simple scaling rules relating I_s to SLG internal properties and ultimately to the graphene quality. In this work we introduce an intuitive numerical model for SLG saturable absorption and extract simple scaling relations between I_s and SLG dynamical rates, such as electron-electron relaxation rate τ_{e-e}, optical dephasing rate τ_{opt} and low-power absorbance rate a_0. Furthermore, we demonstrate the numerical model by direct simulation of the SLG electron dynamics under intense ps-scale pulses, when SLG is introduced in a Bragg cavity under critical coupling conditions [7-10]. This increases SLG absorption close to 100% amplifying all non-linear and saturation effects, while at the same time making the optical response very sensitive to any deviation from critical coupling. We find extreme pulse shaping, including the incident pulse breaking-up into two or three secondary ones. Such extreme sensitivity, in turn, suggests the use of this device as a diagnosis tool for SLG intrinsic fs-scale processes, by simply measuring the response under intense ps-pulses.

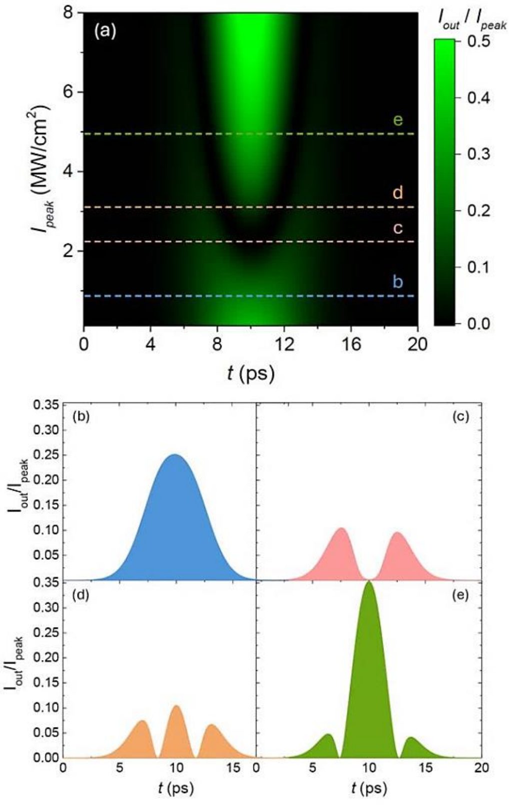

Figure: (a) Temporal colormap of the normalized reflected power density as a function of different peak input power densities. (b-e) Temporal profile of the normalized reflected power density for four different power densities. Specifically, (b) I_{peak} = 0.8 MW/cm^2 resulting to a single output peak, (c) I_{peak} = 2.2 MW/cm^2 resulting to a double peak, (d) I_{peak} = 3.1 MW/cm^2 and (e) I_{peak} = 4.8 MW/cm^2 resulting to triple peaks.

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Orientation-Patterned Gallium Phosphide for Integrated Nonlinear Photonics

K. Pantzas[1], B. Le Corre[1,2], A. Marceau[1,3], G. Beaudoin[1], A. Harouri[1], L. Le Gratiet[1], B. Gerard[4], A. Grisard[3], G. Patriarche[1], Y. Leger[2], S. Combrié[3] and I. Sagnes[1]
[1]*Centre de Nanosciences et de Nanotechnologies, CNRS Université Paris Sacley, 91120, Palaiseau, France*
[2]*Institut FOTON (UMR6082/CNRS-Univ. Rennes-INSA), 35708 Rennes, France*
[3]*Thales Research and Technology, 91767 Palaiseau, France*
[4]*III-V Lab, 91767, Palaiseau, France*

Abstract: Gallium Phosphide has long held promise for integrated nonlinear photonics, owing to its high non-linear figure of merit, broad transparency and compatibility with silicon. However, integration requires very compact crystals and, by extension, very high nonlinear conversion efficiencies. Achieving high conversion efficiencies requires two additional factors: cancelling phase mismatch between the different waves interacting in the nonlinear crystal, and maximizing their spatial overlap. The authors recently developed a process to develop orientation patterned GaP (OP-GaP), a process through which the orientation of the cristal is periodically inverted to ensure quasi-phase matching along the 110 in plane orientation. The OP-GaP crystals were the processed into shallow ridge suspended waveguides. The ridges are 4µm large, 3µm high and 1mm long, and therefore compatible with Silicon Photonic integration. Second harmonic generation experiments from the 1550nm to 775nm were carried out to benchmark the performance of OP-GaP. Despite high propagation losses (~30dB/cm), A record conversion efficiency of 200%/Wcm^2 was demonstrated in these guides [1]. This performance is five hundred times higher than in GaP waveguides without orientation patterned, and only one order of magnitude behind the current state of the art in the mature periodically poled lithium niobate technology (PPLN). Decreasing the losses to about 7dB/cm in this platform will results in conversion efficiencies higher than any current platform. The paper will discuss the fabrication process, additional nonlinear experiments and progress in fabrication of this new platform for integrated nonlinear photonics.

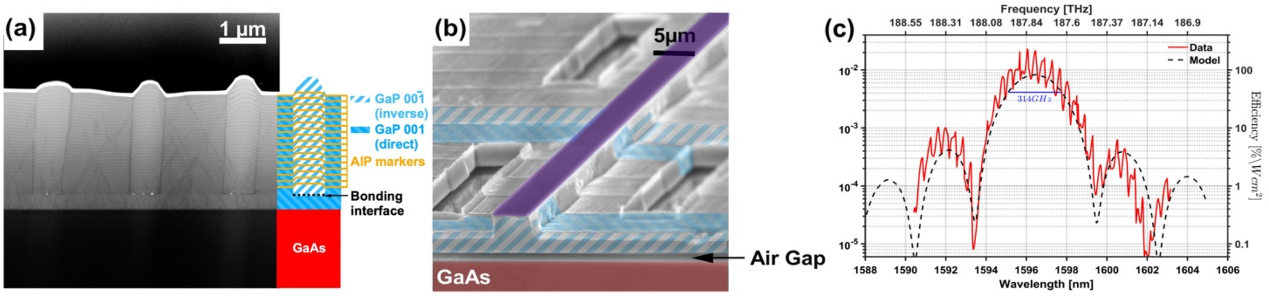

Figure: (a) HAADF-STEM micrograph of OP-GaP, showing the domain inversion along <110>; (b) bird's-eye view of a suspended OP-GaP waveguide; (c) conversion efficiency for SHG in OP-GaP at telecom wavelengths showing a record of 200%/Wcm^2

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Design of a Dual-Metallic Plane Plasmo-Photonic Sensor for Bimodal and Trimodal Interference

P. Zdoupas[1,2], E. Chatzianagnostou[2], L. Damakoudi[1,2], K. Vyrsokinos[1,2]
[1] *School of Physics, Aristotle University of Thessaloniki, Greece*
[2] *Center for Interdisciplinary Research and Innovation, Aristotle University of Thessaloniki, Greece*

Abstract: This work focuses on the design of a plasmo-photonic sensor featuring a dual metallic plane capable of exploiting bimodal or trimodal interference for obtaining either high extinction ratio of the resonant peak or high sensitivity. Fig. 1(a) illustrates a side view of the proposed sensor. The photonic waveguide is composed of 3μm thick SU polymer, while the two plasmonic waveguides are formed by 100nm CMOS compatible Aluminum (Al) spaced apart 750nm and filled also with SU8 polymer. The underclad on the whole platform and the overclad on the photonic waveguides is SiO_2. The upper Al layer is exposed to the surrounding material, and the sensor's sensitivity is evaluated by depositing two water dilutions with nominal refractive indices of 1.312 and 1.313. The sensor's sensitivity remains independent of its length, set at 70 μm in this study.

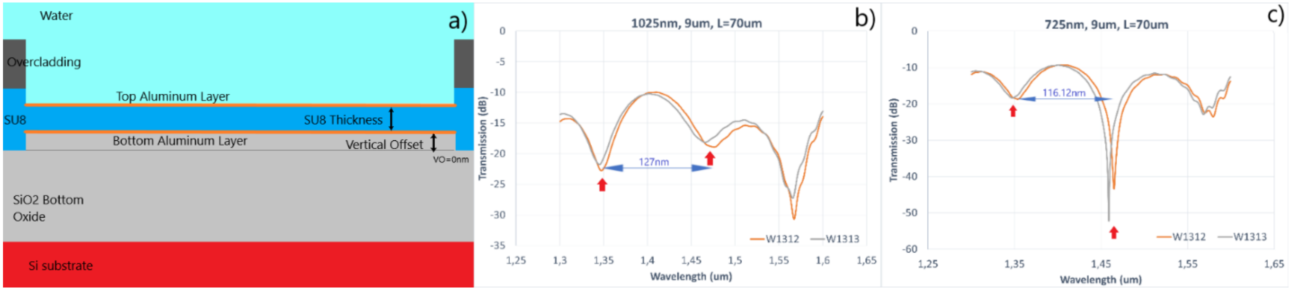

***Figure 1**. a) Side view of the dual metallic plane sensor, b)Spectral response for of the sensor for VO equal to 1025nm where trimodal interference takes place, c) Spectral response of the sensor for VO equal to 725nm that is leading to bimodal interference.*

The vertical offset (VO) of the slot, formed by the two Al layers, from the bottom side of the photonic waveguide determines the excitation and appearance of bimodal or trimodal interference at the output waveguide. When the VO is set to 1025 nm, all three modes i.e. upper, slot, and bottom are excited and propagate at the top Al layer, within the slot, and at the bottom Al layer, respectively, with nearly equal intensities. This configuration results in extremely high sensitivity values of approximately 10,410 nm/RIU, but with an extinction ratio of only 3.3 dB for the dip at 1.47 μm, as shown in Figure 1(b). By altering the VO of the plasmonic waveguides to 725 nm, only the upper and slot modes are excited, leading to a classical bimodal interferometer with an output spectral response illustrated in Figure 1(c). Under the same sensing conditions and for the same resonant peak, the sensitivity decreases to 6,180 nm/RIU, but the extinction ratio surges to 31.5 dB, due to the interference of only two modes with almost equal power.

Organic photovoltaics with efficiencies exceeding 20%

Thomas D. Anthopoulos[1]
[1]Henry Royce Institute, Photon Science Institute, Department of Electrical and Electronic Engineering, The University of Manchester, Alan Turing Building, Oxford Road, Manchester M13 9PL (UK)
E-mail: thomas.anthopoulos@manchester.ac.uk

The recent rapid progress in improving the power conversion efficiency (PCE) of organic photovoltaics (OPVs) has been mainly driven by significant advancements in synthesising new materials and reducing performance losses associated with traditional cell structures. As the PCE values of state-of-the-art OPVs are quickly approaching 20%, the importance of cell engineering, such as the active layer, interfaces, and light management, becomes even more crucial and, in some cases, determines the ultimate cell performance. In this presentation, I will discuss our most recent research, focusing on practical strategies for increasing the PCE of OPVs above 20%. Firstly, I will talk about the use of innovative charge-extracting interlayers and the numerous benefits they offer for use in next-generation OPV products. I will also highlight our latest advancements in utilising molecular electronic dopants to enhance the PCE and show how their combination with the aforementioned innovative interlayers and appropriate cell structures can enhance material utilisation and overall device sustainability while keeping the PCE at record levels.

Materials design and atomistic modelling of perovskites for energy generation applications.

G. Volonakis
Institut des Sciences Chimiques de Rennes, ENSCR, INSA Rennes, CNRS, Université de Rennes.

Over the last decade we have witnessed the rise of lead-halide perovskites for optoelectronic applications such as photovoltaics, sensors and light-emitting diodes. In the first part of this talk I will briefly showcase recent efforts towards new materials that are alternatives to traditional lead-halide perovskites, for which computational design approaches from first-principles have been extensively successful and revealed a series of new compounds within the so-called halide double perovskites family. I will outline the computational design strategy that led to the synthesis of these compounds, and particularly focus on the insights we get from first-principles calculations to facilitate the synthesis, improve their opto-electronic properties and in-silico identification of compounds with properties similar to lead-halide perovskites.

Moreover, I will overview our most recent results on the electronic structure of prototypical structures of layered halide perovskites, vacancy ordered double perovskites, and low dimensional halide perovskite-like materials. I will present the key details of their electronic structure for each type of system that define their experimentally observed optical properties and achieved performances. These results show how well (or how bad) these different types of materials can perform for different opto-electronic applications ranging from indoors and outdoors PV, light emitters. Furthermore, I will present results the substitutional engineering for the class of halide double salts most promising for low-light PVs. Finally, I will focus on our latest state-of-the-art ab initio calculations of the charge carrier transport properties when comparing three-dimensional ABX3 and layered halide perovskites. Our results explore directly the effects of structural dimensionality on the carrier mobilities of a selection of prototypical layered perovskites and identify the importance of the intrinsic carrier density in layered compounds to the exhibited transport properties.

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- **G Volonakis**, N Sakai, H Snaith, F Giustino The Journal of Physical Chemistry Letters 10, 1722 (2019)

Leveraging Molecular Architecture to Design High-Performance Single-Ion Polymer for Energy Storage

Georgia Nikolakakou,[1,2] Christos Pantazidis,[3] Georgios Sakellariou,[3] Vasilis M., Papadakis,[1] Georgios Kenanakis,[1] Benoit Loppinet,[1] Emmanouil Glynos,[1,4]

[1]Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, P.O. Box 1385, 711 10 Heraklion, Crete, Greece
[2]Department of Chemistry, University of Crete, P.O. Box 2208, 710 03 Heraklion, Crete, Greece
[3]Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografrou, 15 771 Athens, Greece
[4]Department of Materials Science and Technology, University of Crete, P.O. Box 2208, 710 03, Heraklion, Crete, Greece
Email: eglynos@iesl.forth.gr

Abstract:
The development of single-ion solid polymer electrolytes (SI-SPEs) with high ionic conductivity hold the key for the realization of safe, long-lasting, high-energy batteries. Despite the considerable research effort in SI-SPEs, the primary challenge that remains is the development of materials with a cation transference number close to unity and good mechanical properties without sacrificing ionic-conductivity. Here we introduce the use nanostructured polyanionic particles as additives to low molecular weight, liquid PEO for the synthesis of nanostructured SI-SPEs that shows a remarkably decoupling between the antagonistic properties of ion conductivity and mechanical behavior. The particles are composed of poly(styrene-4-sulfonyltrifluoro methylsulfonyl) imide lithium, PSTFSILi, arms that complement longer, ion conducting, poly(ethylene oxide), PEO, arms, $(\mathrm{PSTFSILi})_n(\mathrm{PEO})_n$, where $n \approx 22$, as single-ion SPEs. Due to the proposed macromolecular design approach, the polyanion particles are well dispersed for wt% ≤ 55 that enables the formation of a nanostructured single-ion electrolyte with highly interconnected channels composed of liquid PEO that promotes ion conductivity via cation diffusion. Noticeably, while the ion conductivity remains fairly unaffected and close to 10^{-5} S/cm for wt% ≤ 55, the shear modulus, G', monotonically increases by more than 5 orders of magnitude with increasing wt%. These features reveal that the proposed macromolecular design approach offers news means to designed SI-SPEs for the realization of high-energy, safe to use lithium metal batteries

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Polymeric materials for OPVs: Synthetic and LCA perspectives

K.C. Andrikopoulos[1], C. Anastasopoulos[1], A.K. Andreopoulou[1,2], J.K. Kallitsis[1,2]
[1]Department of Chemistry, University of Patras, GR-26504 Rio-Patras, Greece
[1]FORTH/ICE-HT, GR-26504 Rio-Patras, Greece

Abstract:

Organic solar cells have been at the forefront of research efforts to provide a greener solution for the harvesting of solar energy. The active layer of organic solar cells comprises of a semiconducting electron donor and an acceptor such as a fullerenic derivative. However, due to concerns over the stability, cost, and sustainability of fullerenic materials, much effort has been devoted to substituting these materials with polymeric non-fullerene acceptors (NFAs)[1]. Another concern is the synthetic procedures towards the polymeric materials used in the active layer of OPVs, which usually call for toxic reactants such as stannyl derivatives, used in well-established methodologies for polymerizations.

Here we present our efforts to employ the direct arylation polymerization (DArP) method[2], towards fully conjugated polymeric donors, as a more sustainable alternative since no toxic intermediates are required as monomers. With various modifications of the monomers used, we show the control over the morphological, spectral and electrochemical properties of the polymers. Polymeric NFAs are also synthesized, based on perylene and benzothiadiazole derivatives[3], showing controllable absorption profiles. Lastly, the overall environmental footprint of the synthesis of these materials for OPV modules is addressed via life-cycle analysis (LCA) and the results are compared to benchmark PSC modules, that are their direct competitors in the third generation of Photovoltaic technologies[4].

Acknowledgements

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Photochemical activity of WO_{3-x} inverse opal film photoelectrodes

M.-A. Apostolaki[1], E. Sakellis[1, 2], V. Likodimos[1]

[1] Department of Physics, National and Kapodistrian University of Athens, University Campus, 15784 Athens, Greece
[2] Institute of Nanoscience and Nanotechnology, National Centre for Scientific Research "Demokritos", Agia Paraskevi, 15341 Athens, Greece

Structuring semiconductor metal oxides (MOs) in the form of photonic crystals (PCs) attracts particular interest as a promising approach for the development of efficient photoelectrodes exploiting the synergy of slow-light trapping and material's composition [1]. In this study, WO_3 photonic crystal films in the form of macroporous inverse opals were deposited via the co-assembly of monodisperse polymer spheres with ammonium metatungstate aqueous precursor on FTO substrates with optimal band gap [2]. The photonic films were reduced by the acid-induced-metal-reduction (AIMR) method [3] using a metal foil and varying the reaction time in order to develop non-stoichiometric WO_{3-x} phases and generate localized surface plasmon resonance (LSPR) effects by introducing oxygen vacancy defect states into the band gap of WO_3.

Reduced films exhibited decreased reflectance in the visible range, as shown in Fig. 1, which shifted to shorter wavelengths with increasing reduction time, indicating the broadening of LSPR absorption in WO_{3-x} electrodes with increasing W^{5+} concentration. The photonic films were evaluated on photocurrent generation in aqueous $NaHCO_3$ electrolyte under UV–visible irradiation. The reduced WO_{3-x} photoelectrodes exhibited much higher photocurrent density than the pristine WO_3 due to the combination of enhanced light harvesting by slow photons and the excitation of LSPR (Fig. 2), while optimal performance was achieved by controlling the level of oxygen deficiency.

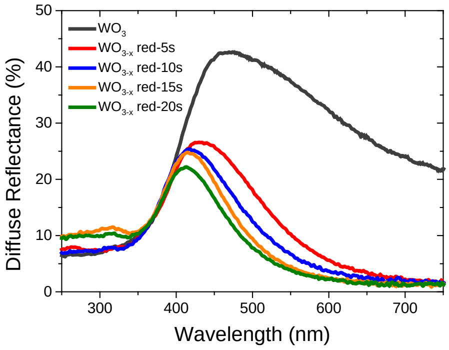

Figure 1 Diffuse reflectance spectra of WO_{3-x} electrodes for different reduction times.

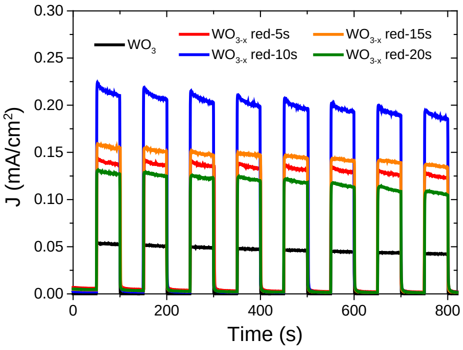

Figure 2 J vs t curves under chopped light for the WO_{3-x} electrodes at 1.23 V vs RHE.

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2D semiconductors: a platform for ultrafast photonics

Giulio Cerullo,[1,*] Stefano Dal Conte,[1] Armando Genco,[1] and Chiara Trovatello[1,2]

1 Dipartimento di Fisica, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133, Milano, Italy

2 Department of Mechanical Engineering, Columbia University, New York, NY, 10027, USA

*giulio.cerullo@polimi.it

Abstract

Layered materials are solids consisting of crystalline sheets with strong in-plane covalent bonds and weak van der Waals out-of-plane interactions. These materials can be easily exfoliated to a single layer, obtaining two-dimensional (2D) materials with radically novel physico-chemical characteristics compared to their bulk counterparts. The field of 2D materials began with graphene and quickly expanded to include semiconducting transition metal dichalcogenides (TMDs). 2D semiconductors exhibit very strong light-matter interaction and exceptionally intense and ultrafast nonlinear optical response, enabling a variety of novel applications in optoelectronics and photonics. Furthermore, stacking 2D materials into heterostructures (HS) offers unlimited possibilities to design new materials tailored for applications. In such HS the electronic structure of the individual layers is well retained because of the weak interlayer van der Waals coupling. Nevertheless, new physical properties and functionalities arise beyond those of their constituent blocks, depending on the type, the stacking sequence and the twist angle of the layers.

This talk will review our recent studies on the ultrafast non-equilibrium optical response of TMDs and their HS. Using high time resolution ultrafast transient absorption (TA) spectroscopy, we monitor the ultrafast onset of exciton formation in TMDs [1] and the dynamics of strongly coupled phonons [2, 3]. Using helicity resolved TA spectroscopy we time-resolve intravalley spin-flip processes [4]. In HS of TMDs we measure ultrafast interlayer hole transfer [5], interlayer exciton formation [6] and use two-dimensional electronic spectroscopy to dissect interlayer electron and hole transfer processes [7]. We also show that strong exciton nonlinear interactions can lead to a complete quenching of the Rabi splitting in TMD-based microcavities [8]. The demonstrated ultrafast switching between the strong and weak coupling regimes paves the way for the development of TMD based high speed all-optical circuits and neural networks.

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Exciton-assisted electron tunneling in van der Waals tunnel junctions

Sotirios Papadopoulos[1], Lujun Wang[1], Fadil Iyikanat[2], Yesim Koyaz[3], Shengyu Shan[1], Jing Huang[1], Ronja Khelifa[1], Takashi Taniguchi[4], Kenji Watanabe[5], F. Javier García de Abajo[2], Lukas Novotny[1]

[1]Photonics Laboratory, ETH Zürich, Zürich, Switzerland.
[2]Institut de Ciències Fotòniques (ICFO), The Barcelona Institute of Science and Technology, Castelldefels, Spain
[3]Photonic Systems Laboratory, EPFL, 1015 Lausanne, Switzerland
[4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan.
[5] Research Center for Functional Materials, National Institute for Materials Science, Tsukuba, Japan.

Abstract: Van der Waals heterostructures have shown great potential for optoelectronic and photonic applications. By stacking atomically thin materials like graphene, hexagonal Boron-Nitride (hBN) and transition metal dichalcogenides, (TMDs), optical sources and photodetectors can be realized. Despite the overall progress, our understanding of the physical mechanisms involved in such devices remains incomplete and puts a limit to our capabilities of designing high-performance devices. Here we present our findings on the important role of energy transfer (ET) between tunneling electrons and excitons in understanding and designing efficient optical sources and detectors. We first introduce a light-emitting device (LED) where a monolayer TMD is positioned on-top of a tunnel junction (Fig. 1a). Despite the fact that the TMD is placed outside of the tunneling pathway we show that excitons are efficiently generated solely through optical coupling (Fig. 1b) [1]. We further discuss that, remarkably, such LEDs present peaks in their differential conductance curve which can be attributed to strong interactions with indirect excitons in the TMDs (Fig. 1c). Additionally, we explore ET effects that lead to overbias excitonic light emission through a two-electron process [3]. Finally, we present our latest results where we employ a monolayer WS_2 flake, that acts as a light harvesting antenna, on-top of a photodetector to demonstrate an 18-fold responsivity enhancement, based on the principle of ET. Collectively, our work expands our understanding of van der Waals devices by revealing the crucial role of ET in the design and performance of optoelectronic devices.

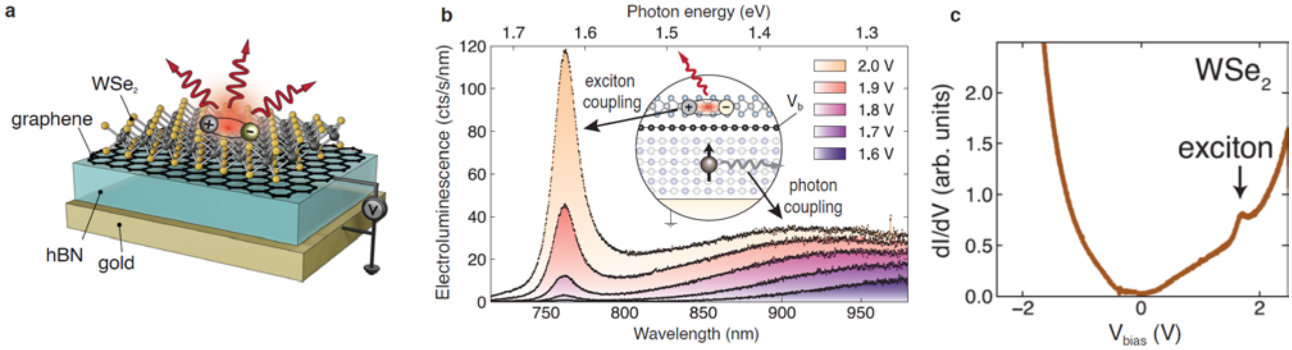

Figure 1: **Exciton-assisted electron tunneling in van der Waals tunnel junctions**. **a.** A light emitting device composed of a TMD on top of a graphene-hBN-gold tunnel junction **b.** Excitonic light emission is observed despite the fact that the TMD is placed outside of the tunneling pathway [1] **c.** Conductance measurement of the device shown in a. Exciton-electron interactions manifest themselves as resonant peaks [3].

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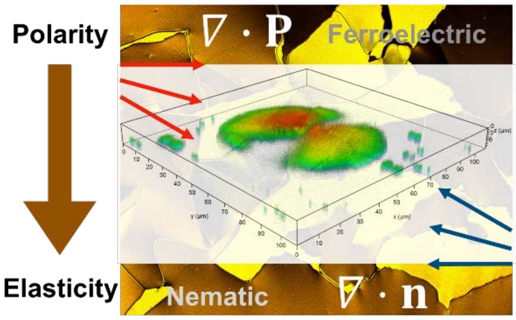
Magneto-optical and Nonlinear-optical Behaviour of a Room-Temperature Ferroelectric Nematic Phase

E. E. Zavvou[1,3], M. Klasen-Memmer[2], A. Manabe[2], M. Bremer[2] and A. Eremin[3]
[1]Department of Physics, University of Patras, 26504 Patras, Greece
[2]Electronics Division, Merck KGaA, Darmstadt, Germany
[3]Otto von Guericke University Magdeburg, Institute of Physics, Dept. Nonlinear Phenomena, Magdeburg, Germany

The recent experimental demonstration of spontaneous macroscopic polar order in a nematic phase composed of rod-like dipolar molecules has sparked immense research interest in the field of liquid crystals [1–4]. Ferroelectric nematics exhibit spontaneous electric polarisation, comparable in magnitude to that of solid ferroelectrics, while retaining 3D fluidity. The spontaneous inversion symmetry breaking within the Ferroelectric Nematic phase (N_F) is accompanied by the formation of macroscopic ferroelectric domains separated by domain walls, in close analogy to solid ferroelectric and ferromagnetic systems. Their remarkable physical properties, such as the huge values of the dielectric permittivity, pyroelectric and second-order nonlinear optical coefficients [2,5–8], render ferroelectric nematogens promising for the realisation of a broad range of high-impact applications [9,10].

The successful exploitation of nematic liquid crystals in a variety of applications, including the display technology, roots at the facile manipulation of the average molecular orientation (director) with external stimuli. Reasonably, studies on the elastic properties of ferroelectric nematics and the implications arising from the direct coupling of spontaneous polarisation to director deformations are of utmost interest. This work comprises an investigation of the behaviour of a room-temperature Ferroelectric Nematic phase in external electric and magnetic fields. The polar order within the N_F phase is established through Second Harmonic Generation studies with the aid of Confocal Laser Scanning Microscopy. The director reorientation is explored in a magnetic field through the combination of optical transmission and dielectric spectroscopy measurements. The experimental findings along with a developed model, capable to describe the director reorientation in a magnetic field, suggest that the ferroelectric nematic phase is much less susceptible to splay than to twist deformation [11]. The strong splay rigidity of the N_F phase is a consequence of the electrostatic self-interaction of spontaneous polarisation, avoiding the polarisation splay.



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Study of the thermal decomposition of ammonium tetrathiomolybdate, $(NH_4)_2MoS_4$), in H_2 and H_2O media by quasi in-situ photoelectron spectroscopy (XPS/UPS).

Labrini Sygellou [1]
[1]Institute of Chemical Engineering Sciences (ICE-HT), Foundation of Research and Technology, Hellas, P.O. Box 1414, 26504 Rio Patras, Greece

Abstract: Molybdenum disulphide, MoS_2, is a two dimensional material constituted from several S–Mo–S planes bonded together by weak van der Waal forces. In the recent years, with the development of preparation methods, MoS_2 has been established as an exceptional material for conventional catalytic, photocatalytic, electrocatalytic and sensing applications. A variety of preparation methods provide the ability to increase the active sites such as edges, boundaries, sulphur vacancies, to activate the basal plane and to tune the band gap. Thermal decomposition of ammonium tetrathiomolybdate $(NH_4)_2MoS_4$) is a common and inexpensive method for fabricated layered MoS_2 of controlled thickness. Here, we report a systematic study of the annealing of $(NH_4)_2MoS_4$) as a function of the reduction atmosphere. The $(NH_4)_2MoS_4$) solution on ITO substrates were annealed at temperatures between 150 °C and 550 °C for 10 min in different atmospheres, such as H_2O, H_2, in 1 atm and ultra high vacuum. The effects of the annealing conditions on the on surface chemistry, elemental composition and the electronic properties of MoS2 films were investigated using quasi in situ X-ray and ultraviolet photoelectron spectroscopy (XPS/UPS). We show that thermally reduced $(NH_4)_2MoS_4$) obtained under oxidic, reducing or inert atmospheres results in MoS_2 films at different temperatures. We show that H_2O induces the formation of Mo oxy-sulfides and oxides increasing the ionization potential. Conversely, H_2 promotes the thermal decomposition of $(NH_4)_2MoS_4$), to MoS_2 at low temperatures, while metallic molybdenum is formed. These results highlight the important role of the heating medium on the temperature at which the thermal decomposition of $(NH_4)_2MoS_4$), takes place for the formation of MoS_2 and lay the foundation for understanding the surface chemistry in combination with electronic properties (work function, ionization potential) as a function of temperature.

Studying 1T-TaS_2 crystals phase transition and charge transfer phenomena at interfaces with perovskites

G. Chatzigiannakis[1,2], A. Soultati[1], S. Gardelis[2], M. Vasilopoulou[1]

[1]*Institute of Nanoscience and Nanotechnology, National Centre of Scientific Research Demokritos, 15341 Agia Paraskevi, Athens, Greece*
[2]*Department of Physics, National and Kapodistrian University of Athens, Panepistimiopolis Zografos, 15784 Athens, Greece*

Abstract:

Tantalum disulfide (1T-TaS_2) is a distinguished 2D transition metal dichalcogenide (TMD) with unique electronic properties including charge density wave (CDW) states and Mott insulating phases upon cooling. The manipulation of these phases by using easy to implement and stable methods to reveal hidden metallic states remains challenging. On the other hand, halide perovskites (HPs) are emerging as a unique class of materials that have already led to breakthroughs in performance of solar cells and light-emitting diodes (LEDs). However, the heavy p-type self-dopance and the high defect density of lead-free HPs deteriorate the performance and stability of perovskite optoelectronic devices. The combination of 1T-TaS_2 with HPs is proposed as a viable solution to overcome these issues by transferring carriers to the interface.

In this work, we studied phase transition of 1T-TaS_2 nanocrystals and bulk crystals as a function of cooling rate by carrying out electrical and structural characterization. In the case of bulk crystals, electrical measurements show an abrupt increase in resistance upon cooling regardless of the cooling rate. In the case of nanocrystals, the abrupt increase in resistance is observed only during gradual cooling while the system keeps a low-resistance metallic behavior when cooled down rapidly. In good agreement, XRD measurements reveal structural changes relevant to the phase transition only during the gradual cooling process. Furthermore, the charge transfer between 1T-TaS_2 nanocrystals and HP thin films deposited on 1T-TaS_2 was investigated. Electrical measurements of such heterostructures show increased conductivity compared to pure crystals attributed to charge transfer at the interface as indicated also by X-ray photoelectron spectroscopy (XPS) measurements. Moreover, ultra-violet photoelectron spectroscopy (UPS) measurements reveal a decreased density of states in the valence band of HP which could also benefit the development of high-performance optoelectronic devices using these hybrid materials.

Acknowledgments

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Photon Energy UpConversion in Organic Semiconductors

P. E. Keivanidis [1]
[1] Device Technology and Chemical Physics Lab
Department of Mechanical Engineering and Materials Science and Engineering
Cyprus University of Technology

Abstract: The photophysical process of triplet-triplet annihilation induced photon energy up-conversion (TTA-UC) is gradually gaining attention as an attractive tool to mitigate the inherently narrow absorption profile of light-harvesting excitonic systems. [1] Particularly for the case of solar energy-related applications, photoactive layers of excitonic materials suffer by transmission losses that waste a considerable fraction of the incoming light. Likewise, excitonic technologies developed by organic semiconductors are handicapped by their inability for panchromatic light harvesting. This limitation applies to all types of photon-energy driven organic electronic devices (OPVs, organic photodetectors, photocatalysts) but it is also relevant for applications involving solar fuels, wherein the excitonic energy is converted to chemical energy. The use of efficient TTA-UC systems to suppress transmission losses in light-harvesting systems is an appealing prospect to establish a sustainable scheme of light management. However, most of the strategies to design efficient TTA-UC solid state interlayers remain incompatible with the fabrication of vertically-configured light harvesting and photonic devices. [2] In addition, the disordered nature of organic materials complicates further the description of triplet exciton diffusion and annihilation in the solid state. [3] In this presentation a novel TTA-UC scheme will be presented [4] for proposing a simple yet effective device engineering protocol that will allow for the effective integration of TTA-UC interlayers in optoelectronic devices.

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Investigation of different Host-Ir(dmpq)$_2$(acac) blended systems for Solution-processable red phosphorescent OLEDs

D Tselekidou[1], K Papadopoulos[1], S Kassavetis[1], A Laskarakis[1], S. Logothetidis[1,2], M Gioti[1]
[1] Nanotechnology Lab LTFN, Department of Physics, Aristotle University of Thessaloniki, GR-54124, Thessaloniki, Greece
[2]Organic Electronic Technologies P.C. (OET), 20th KM Thessaloniki—Tagarades, GR-57001, Thermi, Greece

Abstract: Stable red phosphorescent materials are of high importance in Organic Light Emitting Diodes (OLEDs) technology and applications. A very promising approach involves the use of organometallic emitters, like phosphorescent dopants, an effective emissive layer for OLEDs, which is usually embedded in an appropriate host matrix.

Iridium (III) complexes are the most widely used dopants in Phosphorescent OLEDs because of their high internal quantum efficiency. In this study, four different small molecule host materials, namely 4,4′-Bis(N-carbazolyl)-1,1′-biphenyl (CBP), 1,3-Bis(N-carbazolyl)benzene (mCP), 1,1-Bis[(di-4-tolylamino) phenyl]cyclohexane (TAPC), and tris(4-carbazoyl-9-ylphenyl)amine (TCTA), were doped with Bis(2-(3,5-dimethylphenyl)quinoline-C,N)(acetylacetonato)iridium(III), (Ir(dmpq)2(acac)) with the aim to provide insights into the selection of the best performing host materials for Phosphorescent OLEDs (PhOLEDs).

The net host materials and the Ir(dmpq)$_2$(acac) were studied in terms of their optical and photophysical properties to evaluate the potential energy transfer mechanism from the host materials to the Ir(dmpq)2(acac). The optical and photophysical characteristics of the doped emissive films based on the system Host:Ir(III) complex were examined for three different doping concentrations with the target to achieve pure red-light emission. Following, the doped thin films were implemented as the active layers in OLED devices, formed via the solution deposition method. It was found that OLED devices fabricated for all studied cases emit red light, a characteristic of Ir(dmpq)$_2$(acac), with a maximum wavelength of approximately 620 nm accompanied by CIE Coordinates (0.67, 0.33). By exploring the different combinations between the host and the dopant, as well as the different doping concentrations, we tune the PhOLED emission and device operational stability.

Printable PLEDs as actuators for optical sensing of Rhodamine 6G

K. Papadopoulos[1], D. Tselekidou[1], S. Kassavetis[1], A. Laskarakis[1], S. Logothetidis[1,2], M. Gioti[1]
[1]Nanotechnology Lab LTFN, Department of Physics, Aristotle University of Thessaloniki, 54124, Thessaloniki, Greece
[2]Organic Electronic Technologies P.C. (OET), 20th KM Thessaloniki- Tagarades, 57001, Thermi, Greece

Abstract: In recent years, Organic Light Emitting Diodes (OLEDs) have been considered as the next generation lighting sources. However, a current trend is the application of Polymer based OLEDs (PLEDs) in wearable optical sensors due to their ability to be fabricated, by wet chemistry techniques, such as spin coating or slot die coating, in flexible substrates giving them the advantage of conforming to curved surfaces such as human body.

In this work, we fabricate and extensively study the properties of PLED materials to assess the photophysical, electrochemical, and electrooptical characteristics of printable light-emitting polymers, aiming to ascertain their suitability as emissive layers for wearable PLED applications. NIR-Vis-UV Spectroscopic Ellipsometry (SE), Optical Absorbance, and Photoluminescence (PL) were used to derive the comparative study between the emissive polymers, focused on their optical properties, emission spectral features, and color purity, which are critical factors for PLED-based wearable optical sensors.

Additionally, Cyclic Voltammetry (CV) was employed to determine the HOMO and LUMO energy levels of each material. The fabrication of rigid and flexible light-emitting devices using cost-effective, solution-based methods and facile architecture resulted in high luminance efficiencies, confirmed by Electroluminescence (EL) measurements. Additionally, the tuning of the emission spectral features was achieved by the variation of the emissive layer's thickness, and it was correlated with the thin film's chain packing preferences, for both conjugated polymers.

Finally, the fluorescent dye of Rhodamine 6G was used as an analyte for real life PLED based optical sensing. It was concluded that several factors such as emission wavelength and FWHM, thickness of active material, luminance, and device architecture should be considered for the integration of PLEDs in optical sensing platforms.

Phase Diagram of Polystyrene-*b*-Polyfarnesene Diblock Copolymer System

N. Fotaras[1], M. M. Simon[2], H. Frey[2], G. Floudas[1,3,4]
[1]*Department of Physics, University of Ioannina, 45110 Ioannina, Greece*
[2]*Department of Chemistry, Johannes Gutenberg University, 55128 Mainz, Germany*
[3]*Max Planck Institute for Polymer Research, 55129 Mainz, Germany*
[4]*University Research Center of Ioannina (URCI), Institute of Materials Science and Computing, 45110 Ioannina, Greece*

Abstract: There is an increasing interest in sustainable bio-based polymer materials, like the 1,4-diene monomers isoprene and butadiene. Polyterpenes, based on *cis*-1,4-Polyfarnesene (PFarn), are a promising alternative combining the bio-based background with the abundance of their natural resources. In contrast to polyisoprene (PI), which is a linear polymer, polyfarnesene (PFarn) consists of three isoprene units forming a branch structure similar to this of a bottlebrush-like polymer. This architectural difference leads to a “chain thickening”, which affects both the local and the global (chain) dynamics. As a result, there is an increase in entanglement molar mass, from 5 kg·mol^{-1} for PI to 50 kg·mol^{-1} for PFarn, and the packing length from 3.1 Å to 6.3 Å, respectively [1]. Herein, we report the study of self-assembly (SAXS), viscoelastic properties (Rheology) and dynamics (Broadband Dielectric Spectroscopy), of the PS-*b*-PFarn diblock copolymer over the entire composition range from 0.1 to 0.9 polyfarnesene volume fraction (f_{PFarn}). The phase diagram of the diblock system is established comprising of classical (spheres, cylinders, lamellae) and non-classical (double gyroid) microphases, without any conformational asymmetry ($\alpha_{PS} \approx \alpha_{PFarn}$), resulting in an almost symmetric phase diagram. SAXS and Rheology have been employed to locate the order-to-disorder transition temperature (T_{ODT}) and to extract the segment-segment interaction parameter (χ_{AB}). The later has been estimated both by MFT and Fluctuation Corrections. The diblock structure of PS-*b*-PFarn influences the dynamics, with the dielectric loss curves revealing two segmental processes one for each component respectively. Another segmental processes, is also present, related to the side group of PFarn accompanied by a very weak broad process associated with the PFarn normal mode. The influence of the PS-PFarn interface on the global dynamics for the symmetric systems (lamellae microphases) has also been studied [2,3].

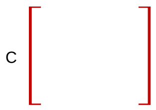

Figure 1. Chemical structure of the diblock copolymer PS-b-PFarn.

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Polymorphism and Heterogeneity in ethanol/water mixtures

V. Moschos[1] and G. Floudas[1,2,3]

[1]Department of Physics, University of Ioannina, 45110 Ioannina, Greece
[2]Max Planck Institute for Polymer Research, 55128 Mainz, Germany
[3]University Research Centre of Ioannina (URCI) - Institute of Materials Science and Computing, 45110 Ioannina, Greece

Aqueous solutions of low-end aliphatic mono-alcohols, such-as the 1-propanol/water mixture, are model systems for studying hydrophobic hydration phenomena and hydrophobic interactions that give rise to local-nano-heterogeneity [1], [2]. Ethanol/water mixtures are of particular interest due to the peculiar polymorphism ethanol exhibits; pure ethanol can be prepared as an amorphous solid, a *bcc* plastic crystal or in fully ordered crystalline state (monoclinic) [3]. By combining structural (XRD), thermodynamic (Differential Scanning Calorimetry, DSC) and dynamical probes (Broadband Dielectric Spectroscopy, BDS), the complete phase diagram of the binary system is established, comprising of different states of ethanol, liquid water, hexagonal ice and different hydrates [4]. The phase diagram is discussed in terms of four regimes; three having in common a droplet arrangement of the minority component and one (ethanol-rich) where ethanol and water are molecularly mixed. Moderately confined water droplets crystallize via homogeneous nucleation well within *No Man's Land* [5]. By probing the dynamics of the mixture over an extended frequency and temperature range, different relaxation processes are identified associated, either with the dynamics of pure ethanol (Debye-like and α-process) or with the dynamics of the different clathrates and interfaces. In equilibrium and non-equilibrium effects are examined by implementing different thermal protocols (slow and fast cooling rates respectively). Differences and similarities of the ethanol/water phase diagram are discussed with respect to the 1-propanol/water binary system, where hydrophobic interactions dominate.

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Preparation and Characterization of Two-Dimensional Nanostructures from Iron Minerals and Study of Their Reinforcement with Metals.

P.T.Kokkinopoulou[1], G. Papathanidis, V. Papantoniou, E. Letsiou, E. Topoglidis, V.I. Georgakilas
[1]*Materials Science Department, University of Patras,*
26504 Patras, Greece

Abstract:
Hematite is a natural mineral that could be found in sedimentary or volcanic format but can be also produced in a laboratory as a final product of oxidation of iron oxides or iron hydroxides. Its use is spread from jewelry to medicine. In the previous years it had been studied for its photocatalytic action as a semiconductor in the splitting of water in order to produce hydrogen. So recently, a study has begun for its use for the development of two-dimensional materials. In this project, hematite minerals and specularite have been used to download two-dimensional nanostructures. The production process began with the pulverize of the mineral into smaller grains, followed by its sonification treatment using the proper organic solvents or water solutions for the exfoliation of the bulk material in nanoplatelets. The role of the organic solvents as well as the conditions of the treatment was studied in a relation with the main characteristics of 2D nanostructures like UV-Vis light absorption, energy gap and the yield of their exfoliation. The aim of the nanostructure doping with the metal atoms or other nanoparticles, aims toward the improvement of the properties of the materials which are connected to its utilization in electrocatalytic and the photoelecrocatalytic split of water respectively. Finally, the study of the materials, was performed using instrumentation available at our university, such as a) X-ray Diffraction analysis spectroscopy, b) UV – Vis absorption Spectroscopy, c) Cyclic Voltammetry as well as technical microscope analysis such as Scanning Electron Microscopy.

CARBON DOTS’ UNUSUAL OPTOELECTRONIC PROPERTIES IN SILICA AEROGELS

A. Tiron-Stathopoulos[1] and K. Dimos[1]
[1] Department of Materials Science, University of Patras, GR-26504 Patras, Greece

Over the past few years, there has been a lot of research focused on finding new synthesis pathways and applications for aerogels across a range of fields, mostly because of the distinctive properties they exhibit such as outstanding thermal insulation combined with low density and high surface area [1]. Several applications benefiting from these unique properties have been proposed and some of them have been already commercialized like thermal insulation in aerospace applications [2], and others are still under development, like drug delivery [3], gas sensing [4], biosensors [5], and energy storage [6]. On the other hand, carbon dots represent a novel class of functional nanoparticles that combine low-cost and effective synthesis with advantageous optical characteristics such as steady and tunable photoluminescence [7,8]. Carbon dots can be doped with a variety of heteroatoms to modify their intrinsic properties, including phosphorus, nitrogen, sulfur, and boron [9]. The combination of these two types of materials gives rise to composite aerogels. Composite aerogels integrate the characteristics of the aerogel matrix along with the ones by the inclusions, which may be diverse materials in different forms.

In this work, we present the preparation of fluorescent composite silica/carbon dot aerogels, we study their physical properties, and we focus on their optical response. The method we use to prepare the composite aerogel is the classical sol-gel process using tetraethyl orthosilicate as silica precursor, followed by CO_2 supercritical drying. Comparing the resultant aerogel to the pure carbon dots in solution, it shows a variety of optoelectronic features, including an excitation-dependent emission and a unique blue-shift for excitation focused in the UVB area. Additionally, the aerogel is highly porous and crack-free. The unfamiliar optoelectronic properties of the carbon dots in the aerogel are discussed and are attributed to several factors linked to the silica matrix.

KEYWORDS: Silica aerogels, carbon dots, fluorescent aerogels, composite aerogels, blue-shift

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Highly-Robust Stacked-Memristor based on Perovskite/Molybdenum Oxide-Sulfide Heterostructure

A. Soultati[1], A. Verykios[1], G. Calemai[1,2], G. Chatzigiannakis[1,3], D. Davazoglou[1], K. Aidinis[4,5], M. Vasilopoulou[1]

[1]Institute of Nanoscience and Nanotechnology (INN), National Center for Scientific Research Demokritos, 15341 Agia Paraskevi, Athens, Greece
[2]Department of Physics, University of Patras, 26504 Patra, Rio, Greece
[3]Solid State Physics Section, Physics Department, National and Kapodistrian University of Athens, Panepistimioupolis, 15784 Zografos, Athens, Greece
[4]Department of Electrical and Computer Engineering, Ajman University, P.O. Box 346, Ajman,United Arab Emirates.
[5]Center of Medical and Bio-Allied Health Sciences Research, Ajman, United Arab Emirates

Abstract: Halide organic-inorganic perovskites (HOIPs) are a promising class of materials for neuromorphic computing and processing systems demonstrating a variety of resistive switching (RS) mechanisms. HOIPs have been used as active layers in two- and three-terminal synaptic devices reporting high performance in metrics of speed and energy consumption. However, halide perovskites suffer from poor ambient stability and reproducibility. In this work, a highly-robust double memristor based on two active layers forming a stacking heterojunction is demonstrated. In particular, the functional layer consisted by a molybdenum oxide-sulfide compound (MoO_3-MoS_2) and a quadruple cation perovskite (RbCsMAFA) deposited on top showing favorable band alignment for the specific application. The double memristor based on the MoO_3-MoS_2/RbCsMAFA heterojunction exhibited impressive and stable resistive switching behavior with ON/OFF ratio of around 10^2, endurance of 100 cycles, high retention of $2•10^4$ s, and high environmental stability maintaining its memristive behavior for 1 month. The space-charge limited current conduction mechanism is dominated by the states within the bandgap of the MoO_3-MoS_2 that could act as traps in the MoO_3-MoS_2/RbCsMAFA heterojunction leading to the switch from ohmic to SCLC conduction in the double memristor. Furthermore, the emulation of the biosynapse behavior was studied including paired-pulse facilitation (PPF), post-tetanic potentiation, and transitions from short-term (STP) to long-term plasticity. The robust device also exhibited good thermal stability maintaining the memristive characteristics at 85°C, as well as good photonic memristive behavior with improved ON/OFF ratio under constant illumination. Our findings prove that the proposed double memristor is a promising candidate for artificial synapses and neuromorphic computing systems.

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DC sputtered ZnO:Al thin films as methane gas sensors

C.-P. Tsichlis[1], E. Gagaoudakis[1], A. Sfakianou[1,2], V. Binas[1,2]
[1]Foundation of Research and Technology - Hellas, Institute of Electronic Structure & Laser (FORTH-IESL), Heraklion Greece
[2]Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece

Abstract: Methane is a colourless and flammable gas that is used worldwide as a fuel for electricity and heating generation and plays important role in driving climate change. It can be explosive when its concentration reaches 5 to 15% in an enclosed area. Thus, there is urgent need to develop methane gas sensors, to monitor its concentration during the production, storage, transportation and use procedures. For that reason, a wide range of material have been used as gas sensing elements for methane detection, including metal oxide semiconductors, carbon-based materials, conducting polymers and other 2-D materials.

In this work, DC sputtered ZnO:Al films, grown at room temperature, were tested against different methane concentrations, at elevated temperatures. from room temperature (25°C) up to 400°C. The structural, morphological and optical properties of the films were examined by X-Ray Diffraction (XRD) technique, Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM) and UV-Vis spectroscopy, while Energy Dispersive Spectroscopy (EDS) was used to determine the stoichiometry of the films.

In Fig. 1, the response of the ZnO:Al films to methane gas of different concentrations is presented. It can be seen that ZnO:Al gas sensors have the ability to detect low concentrations of methane gas, indicating that is a possible candidate material for methane gas sensing applications.

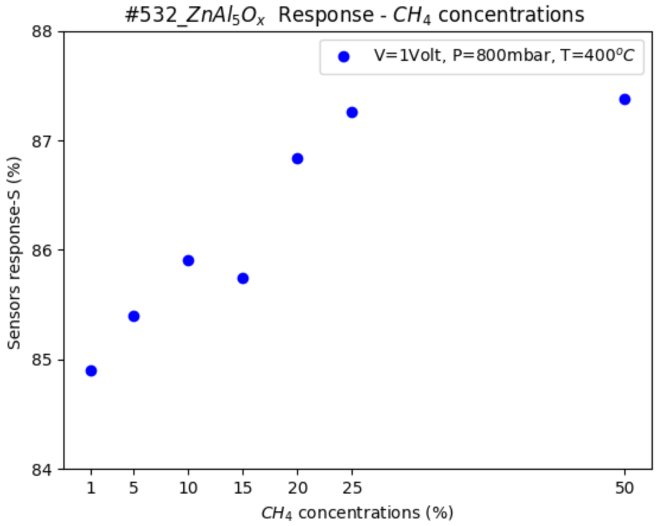

Figure 1: Response of ZnO:Al methane gas sensor against different methane concentrations.

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High dislocation density in iron-doped mullite

Svetlana Ilić, Milica Pošarac - Marković, Aleksandra Šaponjić, Jovana Ruzić

Vinča Institute of Nuclear Sciences, Univeristy of Belgrade, National Institute of the Republic of Serbia, Belgrade, Serbia

Abstract: Iron incorporation in the mullite structure and sol-gel synthesis procedure have a beneficial influence during the mullitization and processing of the material. After formation, this material has significantly improved mechanical properties compared to a pure, undoped mullite. Investigated materials contained various amounts of Fe_2O_3 (3, 6 and 9 wt.%). Vickers hardness and nanoindentation tests revealed that the sample containing 6 wt.% Fe_2O_3 has the highest impact on mechanical properties. However, the value of Vickers hardness near the solubility limit (9 wt% Fe_2O_3) was lower. Such an uncommon finding has been confirmed by more detailed XRD analysis, leading to the calculation of dislocation densities based on structural parameters. The dislocation density in iron-doped mullite has reached the values of ~10^{15} m^{-2}. After nanoindentation tests, the values of hardness and elastic modulus exhibited improvement of these mechanical properties up to 6 wt.% Fe_2O_3 (H = 13.9 GPa; E_r = 178.7 GPa), and also the sample with 9.0 wt.% Fe_2O_3 showed decreasing in hardness and elastic modulus (H = 7.6 GPa; E_r = 154.7GPa). The principal cause may be an increase in the density of defects, primarily dislocations at the crystallite level (~50 nm). Also, many pile-ups were observed around the indents caused by dislocation motions under the applied load.

Sintering behavior of yttrium-doped spinel powder directly synthesized by the solution combustion method

M. Posarac - Markovic[1], A. Saponjic[1], S. Ilic[1]

[1]*Materials Science Laboratory, Vinca Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovica Alasa 12-14,Serbia*

Abstract: Magnesium aluminate spinel, $MgAl_2O_4$, is a well-known structural material with numerous applications across various industries, particularly as refractory materials. It is also utilized in the construction of sensors, ceramic membranes, optical devices, and as a catalyst or catalyst carrier. Doping magnesium aluminate with yttrium ions can lead to better sinterability of nanostructured polycrystalline spinel material by stabilizing the nanostructure against grain growth. Grain growth is inhibited by the addition of dopant, which occupies high-energy sites at the grain boundaries and restricts their mobility. Also, incorporation of larger-sized dopant cations, such as Y^{3+}, into the spinel structure causes lattice strain, which aids in mass transfer and densification and can lead to improvements of hardness, thermal stability and chemical resistance.

$MgAl_{2-x}Y_xO_4$ powders (x=0, 0.02, 0.06, and 0.10) were directly synthesized by the solution combustion method using metal nitrates and a mixture of fuels specified for each metal nitrate used. During a very short synthesis time (about 30 minutes), crystalline spinel powders with approximately 40 nm-sized crystallites were obtained. Prepared powders were consolidated by different uniaxial pressures, 90 MPa and 125 MPa. The sintering behavior of samples sintered at 1300ºC and 1500ºC, with an annealing time of 2 hours, was investigated, and structural and morphological analyses were performed using X-ray diffraction, scanning electron microscopy (SEM), and energy dispersive spectroscopy (EDS).

Enhanced Radiative cooling through Microstructured polymer film fabricated by Nanoimprint lithography

N. Dimogerontaki[1,2], N. Matthaiakakis[2], N. Kehagias[2]

[1] Department of Physics, School of Applied Mathematical and Physical Sciences National Technical University of Athens, Zografou Campus, GREECE
[2]NCSR Demokritos, Institute of Nanoscience & Nanotechnology, P. Grigoriou 27 & Neapoleos Str., 15341 Ag. Paraskevi, Greece

Abstract:

Radiative cooling presents a passive cooling solution by enabling terrestrial objects to emit heat into outer space through the atmospheric transparency window (ATW) in the 8-13 μm wavelength range. This technology focuses on the development of materials engineered to emit radiation effectively in these wavelengths to achieve cooling.

In recent years, this method has been proposed for cooling solar cells, which suffer from loss of efficiency and decreased lifetime due to overheating. Coolers designed for solar cells should possess two key traits:

1. High emissivity in the ATW range to achieve efficient cooling.
2. High transparency in the visible range to allow maximum absorption of solar radiation by the solar cells.

Methods for large-area and cost-effective fabrication like nanoimprint lithography, and exploration of various materials and geometries of photonic structures are crucial in the pursuit of an effective and scalable radiative cooling technology for solar cells.

In this work, we investigate the radiative cooling effect of micro-structured transparent polymer films fabricated by UV-Nanoimprint lithography as promising candidates for effective radiative cooling of solar cells. A UV-curable hybrid organic-inorganic material was chosen for the study due to its characteristics, including high transparency (over 90%) in the visible range and high emissivity within the atmospheric window. The samples were fabricated on silicon wafer substrates. Emissivity measurements as well as temperature measurements are employed to acess the cooling performance of the radiative coolers.

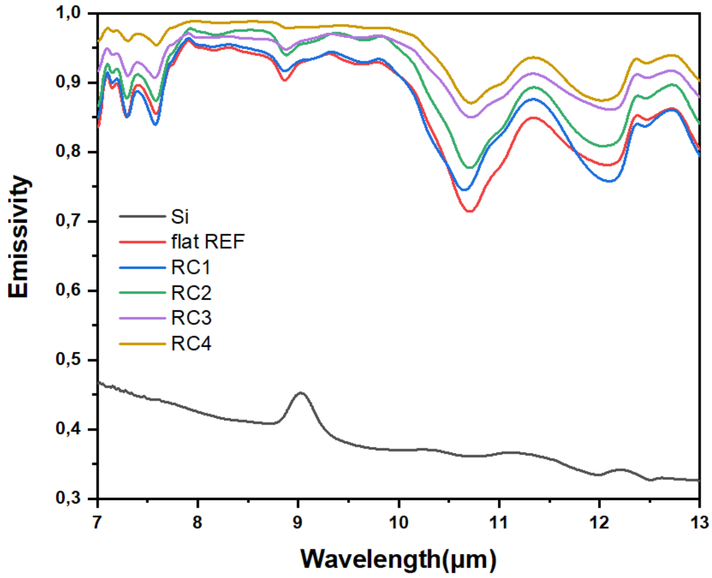

Figure 1 Emissivity measurements in the atmospheric transparency window of bare Silicon (Si), an unstructured reference (flat REF) and different microstructured radiative cooling polymer films (RC1-4)

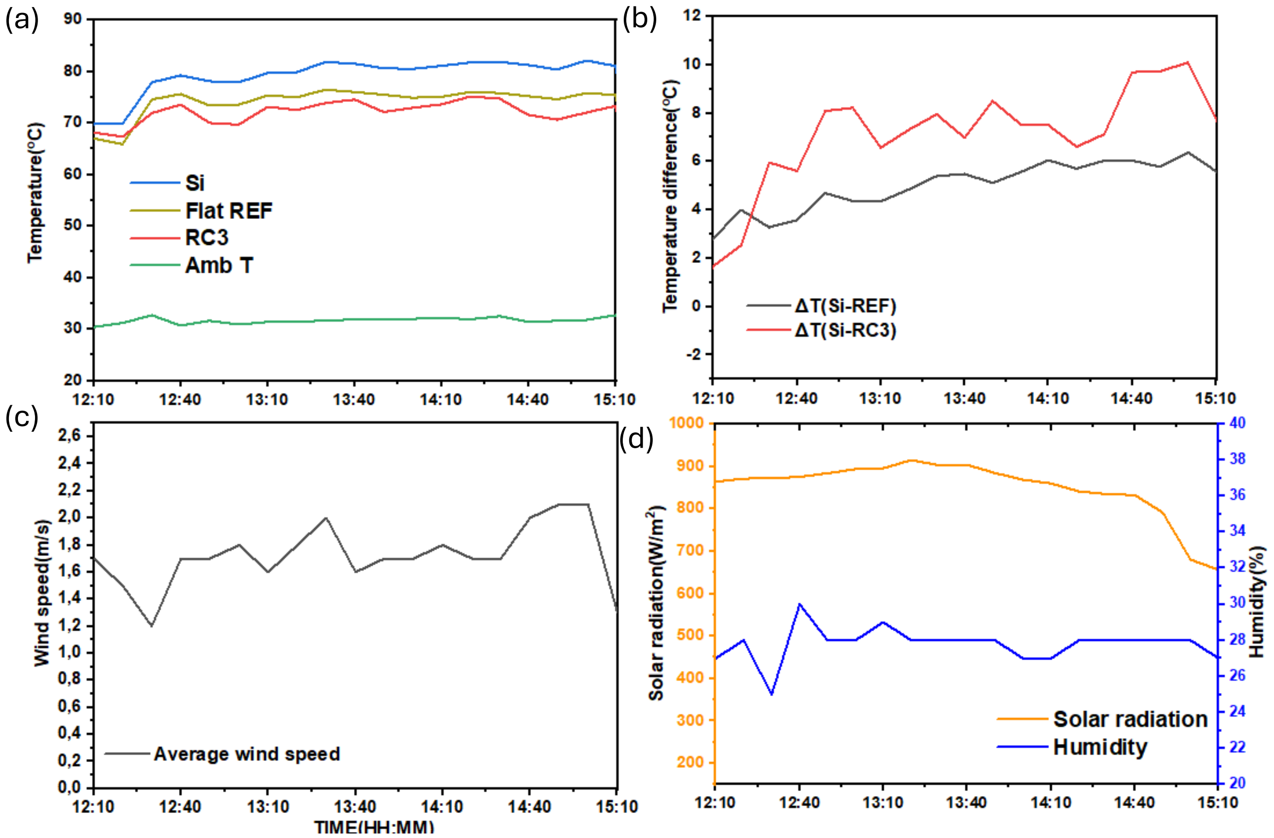

Figure 2 (a) Temperature measurements of the bare Silicon sample, the flat reference and a radiative cooling film during noon hours on June 17 2024. (b) Temperature difference between bare Silicon and the radiative cooler and the bare Silicon and the flat reference. (c) Average wind speed. (d) Humidity and solar radiation.

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A numerical model incorporating machine learning for crack propagation in materials with inclusions

G. Makris[1], K. Kolomvatos[1], F.Sofos[2], T.Karakasidis[2]
[1]*Department of Informatics & Telecommunications, University of Thessaly, 35100 Lamia, Greece*
[2]*Condensed Matter Laboratory, Department of Physics,*
University of Thessaly, 35100 Lamia, Greece

Abstract: The mechanical properties of materials, specifically toughness, and hardness, are affected by the concentration and the geometrical and physical properties of the crystalline inclusions since they influence crack propagation modes. Computer simulation play an essential role in studying crack propagation. Work on a standalone inclusion and semi-analytical model in two dimensions has been developed, and the results are quite similar to the observed behavior. Simulating the collective effect of many inclusions on crack propagation and the impact of concentration, size, and cohesion energies of matrix/inclusion regions is a very complex problem. Since crack propagation is a multiscale phenomenon, macroscopic methods such as Finite Elements and the continuum approach could not accurately describe it. On the other hand, Molecular Dynamics, which simulates materials at the atomic scale, is very computationally demanding.

Thus, we developed a semi-analytical model where the material is represented as blocks of matrix and inclusion areas, each corresponding to a different cohesion energy. Samples with given concentration and nano-inclusion sizes are created, and then the crack is simulated as the breaking of material blocks based on a modified blind walker model. Several crack propagations are simulated, and average quantities, such as the mean crack length, are computed. Then a machine learning methodology is applied, promising further acceleration of simulations when studying complex geometries. Using this approach the effect of crystalline inclusion concentration, the size of the inclusions, and the difference of cohesive energies of the matrix and the crystalline inclusion were investigated. The computational framework could lead to a multiscale computational framework, using as input detailed calculations from DFT for cohesion energies of more complex materials.

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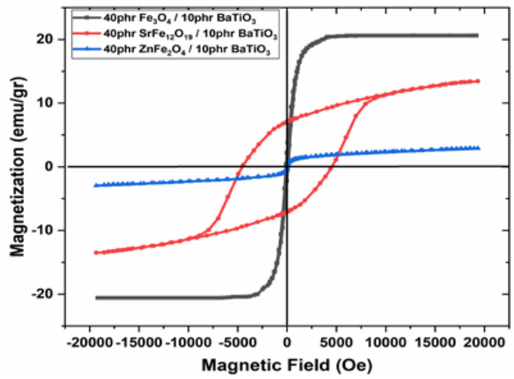
Inducing Magnetic Properties in Polymer Matrix Nanocomposites

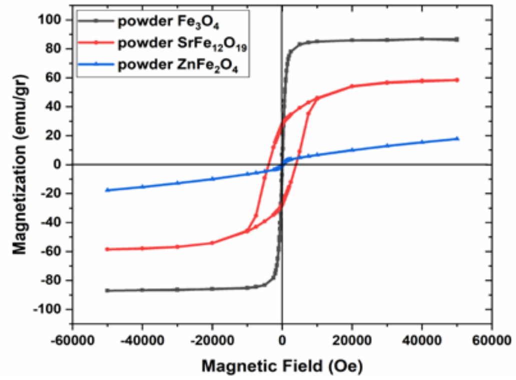
A.C. Patsidis[1], G. C. Manika[1], S. Gioti[1], A. Sanida[1], N. Petropoulos[2], A. Kanapitsas[2], C. Tsonos[2], Th. Speliotis[3], G.C. Psarras[1]
[1]Department of Materials Science, University of Patras, Patras, Greece,
[2]Department of Physics, University of Thessaly, Lamia, Greece,
[3]Institute of Nanoscience and Nanotechnology, NCSR "Demokritos", Athens, Greece

Abstract: Nowadays, polymer matrix nanocomposites are considered as an important class of engineering materials for various technological applications. Epoxy resins are the most popular matrices for the development of advanced composites, since they are characterized by low weight, easiness of processing, flexibility, good wetting and adhesion with the majority of the employed fillers, at low cost. Their properties can be improved by integrating various fillers, which advance their thermomechanical properties, dielectric and electrical response, magnetic properties, and the ability to store and recover electrical energy. By these means, multifunctional performance can be induced by integrating suitable fillers, which exhibit supplementary properties/responses[1-3].

In this study, series of hybrid epoxy nanocomposites with magnetic nanoparticles (Fe_3O_4, or $ZnFe_2O_4$, or $SrFe_{12}O_{19}$) and $BaTiO_3$ have been prepared and studied. Fabricated hybrid systems are able to respond under various loading conditions, exhibiting suitable mechanical/thermal properties, tunable electric conductivity, variable electric polarization/dielectric permittivity, adjustable magnetic response, and thermally induced phase changes. All these responses contribute to the overall multifunctional performance.

Hybrid nanocomposites were characterized by means of Scanning Electron Microscopy (SEM), X-Ray Diffraction (XRD), and their magnetic properties of the hybrid nanocomposites were examined via a Vibrating Sample Magnetometer (VSM) at ambient.





Results imply the successful fabrication of nanocomposites and the fine dispersion of the nano-inclusions. Magnetic particles induce magnetic properties to the nanocomposites, which vary with the type and the amount of the employed magnetic phase. Magnetic saturation and remanence enhance with magnetic phase content. The magnetic type of the filler (i.e., hard/soft/supermagnetic) is induced to the hybrid nanocomposites.

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High performance 4D printed electrothermal actuators with SWCNT segregated structures

Stavros Katsiaounis [3,4], Miron Krassas [1,2], Emmanouil Porfyrakis [1,2], Fivos Simopoulos [1,2], Georgios Kampourakis [1,2], George Karalis [1,5], Lazaros Tzounis [1,2,5], Konstantinos Papagelis [3,4*]

[1]Mechanical Engineering Department, Hellenic Mediterranean University, Estavromenos, 71004, Heraklion, Crete, Greece
[2]Institute of Emerging Technologies, University Research and Innovation Center, HMU, 71410 Heraklion, Crete, Greece
[3]Foundation for Research and Technology Hellas, Institute of Chemical Engineering Sciences, P.O. Box 1414, GR-26504, Patras, Greece
[4]School of Physics, Department of Solid-State Physics, Aristotle University of Thessaloniki, Thessaloniki, 54124, Greece
[5]Printed Electronic Devices of Things P.C. (PDoT), Makrinitsis 122, GR-38333, Volos, Greece

Abstract: U-shaped bimetallic polymer-based electrothermal actuator (ETA) devices were fabricated using Fused Filament Fabrication (FFF) three-dimensional printing (3DP). These devices (referred to as 4D printed bi-metallic ETA devices) feature a bilayer structure of acrylonitrile butadiene styrene (ABS) and conductive thermoplastic polyurethane (cTPU). The cTPU layer is printed with a gyroid micro-architecture, enabling the infiltration of single-walled carbon nanotube (SWCNT) aqueous ink via an automated ink deposition process to enhance conductivity and electrothermal performance. A continuous SWCNT segregated structure forms within the cTPU layer pores, resulting in a significant reduction in internal resistance from approximately 9 KOhm to ~20 Ohm in the 4DP ABS/cTPU/SWCNT ETA device.

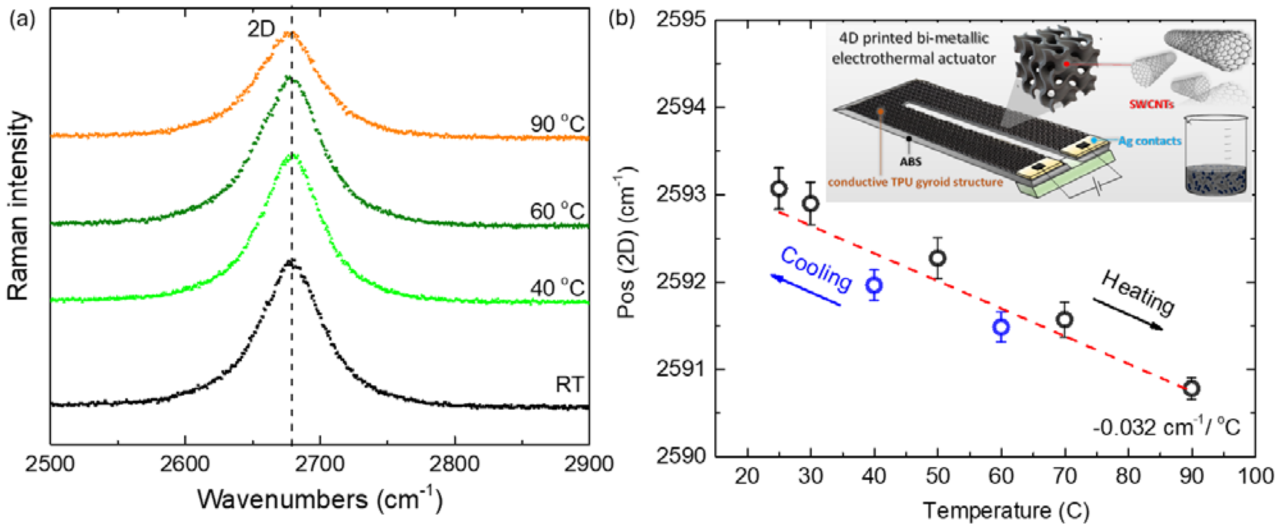

Figure 1. (a) Raman 2D peaks of SWCNTs ink under varying temperatures. (b) Variation of Raman 2D peak position of SWNTs ink as a function of temperature. Inset: 4D printed ABS/cTPU/SWCNT ETA device.

The 4DP ETAs were evaluated for their actuation performance under different applied bias voltages (Vbias) and ON-OFF alternating cycles, with real-time tip displacement measured using a high-resolution camera and dedicated video analysis software. The force generated by the 4DP ETAs was measured with a digital micro-balance, and Infrared thermography (IR-T) images were captured during operation to confirm the electrothermal Joule heating effect.

Raman spectroscopy was used to assess the structural quality and tube diameters of SWCNTs and to observe the temperature-dependence of the recorded Raman modes (20-90 ^{o}C) under cooling and heating

* Corresponding author
Email: kpapag@physics.auth.gr (K. Papagelis)

cycles. In the low frequency regime (100 – 300 cm^{-1}), the radial breathing modes (RBMs) correspond to the coherent vibration of the carbon atoms, where all the tube atoms vibrate radially in phase. From the peak positions of the RBMs, the range of diameters that are in resonance with the excitation energy can be determined (0.87-1.96 nm). In the high-energy region of the Raman spectrum of SWCNTs, two main first-order components are present, resulting from the in-plane C–C carbon displacements parallel and perpendicular to the tube axis, usually labelled as G$^+$ (≈1591 cm^{-1}) and G$^-$ (≈1566 cm^{-1}). Additionally, at ≈2672cm^{-1} (λ=514 nm) the 2D mode appears, which is the second harmonic of the disorder-induced D-band. Upon temperature application, all the aforementioned bands exhibit a red shift with an increase in temperature. The consistent red shift in Raman peaks with increasing temperature confirms the robustness of the nanocomposite under thermal stress, highlighting the potential of our fabricated devices for applications requiring high thermal stability and resilience.

Acknowledgments

THUNDER (Thermal stimuli-responsive 3D printed electroactive polymer nanocomposites towards 4D “programmable” geometries) research project received funding from the Hellenic Foundation for Research and Innovation (HFRI) under the HFRI Greece 2.0 Basic Research Financing Action (Horizontal support of all Sciences) Sub-action II Funding Projects in Leading-Edge Sectors (Project ID Number: 15515).

THUNDER

H.F.R.I.
Hellenic Foundation for Research & Innovation

Greece 2.0
NATIONAL RECOVERY AND RESILIENCE PLAN

ΕΛ.Ι.Δ.Ε.Κ.
Ελληνικό Ίδρυμα Έρευνας & Καινοτομίας

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* Corresponding author
Email: kpapag@physics.auth.gr (K. Papagelis)

Resistive Switching Phenomena in flexible devices based on composite materials, in spot- and grid-like architectures

A. Mourkas[1], A. Dellaporta[1], I. Panagiotopoulos[1],
[1]*Department of Materials Science and Engineering, University of Ioannina, 45110, Ioannina, Greece*

Abstract

Recently, resistive switching devices (RSDs) have emerged as a possible candidate for replacing traditional non-volatile memory devices for in-memory computing, wearable electronics, neuromorphic applications etc. Traditional rigid devices based on inorganic materials have been studied extensively, but the high fabrication cost and the high processing temperatures that are required, resulted in exploring other suitable candidates. Typically, organic materials require lower temperatures (close to room temperature) and a simpler, cost-effective, fabrication. Thus, combining them with inorganic materials leads to hybrid composite materials with good electrical, optical and magnetic properties while maintaining the excellent mechanical capabilities of flexible substrates. Metal Oxides (MOs) such as TiO_2 and ZrO_2 have been studied, among other MOs, for their resistive switching properties. In this work we present a device fabricated with printing techniques, based on the organic material Polyvinyl(4-Phenol), known as PVP, and the MOs ZrO_2 nanoparticles. ITO coated PET substrate is utilized as our bottom electrode. The active layer deposition was carried out by the simple technique of spin coating, while the top electrode (Ag) is deposited via screen printing. The PVP acts as a matrix for the ZrO_2 nanoparticles to prevent unwanted agglomeration, and to extend the mechanical capabilities of the device. Different ratios (0,1:1, 0,25:1, 0,5:1, 1:1) of ZrO_2:PVP have been explored to achieve the optimal blend for the composite material. We prepared two different architectures for the device: a) a grid architecture and, b) a spot architecture. The spot architecture returns a bigger R_{OFF} / R_{ON} value, possibly due to the leakage current from that affects the contacts in the grid architecture.

Micromagnetics of microwave assisted magnetization switching in nanodisks at finite temperatures.

Christos Thanos[1], Ioannis Panagiotopoulos[1]
[1]*Department of Materials Science and Engineering, University of Ioannina, 45110 Ioannina Greece*

Abstract:

Microwave assisted switching of the magnetization (MAS) refers to lowering the switching field by resonantly exiting the processional motion of the magnetic moment using a radio frequency field. This method has attracted a lot of attention lately due to its application in magnetic recording media (“microwave assisted magnetic recording”) to alleviate the conflicting constraints of increased density, high signal-to-noise ratio, writability and thermal stability [1]. In most of the simulations of this process the thermal effects are ignored. Including the thermal effects not only helps towards making more accurate predictions but it is also of great scientific interest as the resonant response is fundamentally different from a thermal one.

Here microwave assisted magnetic switching (MAS) is simulated for CoPt(4 nm)/Co_3Pt(2 nm) 15nm diameter disks nanostructures as a function of microwave frequency, amplitude for different temperatures. The results show that the range of usable frequencies depends sensitively on the amplitude of the RF signal. At the limit between the conditions that lead to switching and the ones that do not, probabilistic switching is observed [2]. The results are discussed using the concept of effective write field derived by Stoner-Wohlfarth model predictions within a frame that rotates with the microwave frequency [1]. Our simulations do not fully concur with this simple approach that predicts an assistance effect proportional to the frequency but almost insensitive to the amplitude microwave field.

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Optimized Processing of NiCuZn-ferrites

S. Zaspalis[1,2], G. Kogias[1], S. Kikkinides[2]

[1]*Laboratory of Materials Technology, Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki, Greece*

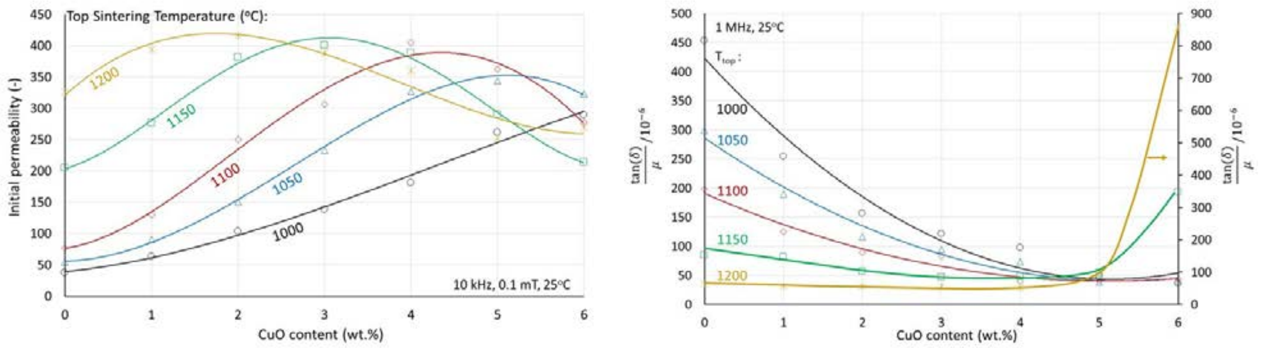
[2]*Laboratory of Inorganic Materials, Chemical Process and Energy Resources Institute, Center for Research and Technology-Hellas, Thessaloniki, Greece*

Abstract:

The main driver for the introduction of Cu in NiZn-ferrites was the necessity for the development of low sintering temperature materials, compatible with the low melting temperatures of the electrode (usually Ag) metals employed in multilayer components. However, Cu is also a very useful additive for the manufacturers of monolithic NiZn-ferrite components. As a raw material, Cu is cheaper than Ni. In addition, the low required sintering temperatures are in favor of lower energy costs.

In this article is reported on the effect of Cu-content in combination with the sintering temperature, on the magnetic permeability and power losses of monolithic iron deficient NiCuZn-ferrite components for power applications at frequencies up to 1 MHz. As found, the main advantage of Cu is not the achievement of better magnetic performance but identical magnetic performance at quite lower sintering temperatures, therefore at lower production cost. As found, there is not one optimum Cu-content, instead there are several combinations of Cu-content and sintering temperature, for optimum magnetic performance (i.e. higher magnetic permeability or lower power losses), among which the materials engineer may choose (see Figure).

At CuO content higher than 5 wt.% and sintering temperatures higher than 1150°C, pronounced microstructural disturbances, due to asymmetric grain growth, result to low permeabilities and high losses. It is suggested that at low CuO contents and low sintering temperatures the densification enhancement may not proceed through Cu-rich phase segregation but through the creation of oxygen vacancies.



Ni as an additive in MnZn ferrites

G. Kogias[1], S. Zaspalis[1,2], V. Zaspalis[1,2]
[1]Laboratory of Inorganic Materials, Chemical Processes and Energy Resources Institute, Centre for Research and Technology-Hellas, 57001 Thermi-Thessaloniki, Greece
[2]Department of Chemical Engineering, Aristotle University of Thessaloniki, University Campus, 54124, Thessaloniki, Greece

Abstract:

MnZn ferrites is the most widespread family of soft ferrite materials with a very broad spectrum of applications in automotive, (micro-) electronics or telecommunications, up to operation frequencies of 1-3 MHz. They are mostly used, in the form of polycrystalline cores, as inductors, transformers or absorbers, although recently they are investigated, in micro- or nano-powder form, for inductive heating, environmental and biomedical applications.

In this article an extensive study is presented on the Ni addition in three subcategories of MnZn ferrites under conditions of constant Mn/Zn ratio and Fe excess, namely i) Group A: low frequency (~100 kHz) power ferrites, ii) Group B: medium frequency (~500 kHz) power ferrites and iii) Group C: high permeability (μ_i ~8000, 25°C) ferrites.

The materials of this discussion are polycrystalline iron excess ferrites of the general formula $(Mn_{1-x}Zn_x)Fe_{2+\delta}O_4$, synthesized by the conventional ceramic method. A mixture of raw materials is prefired, milled, granulated, compacted in specimens of toroidal geometry, and subjected to sintering at elevated temperatures (T), ~1200-1350°C, where the cooling takes place under equilibrium partial pressure of O_2 in order to adjust the Fe^{2+}/Fe^{3+} ratio.

As found, Ni is a useful additive for optimizing the high temperature performance of MnZn ferrites since it increases Curie T (Tc), saturation flux density (Fig.1), magnetic permeability and decreases power losses at T above 100°C. In addition, the addition of Ni increases the resonance frequency and the frequency stability of the initial permeability and partly counteracts the ageing effects caused by Co, when it is present in medium frequency ferrites. The magnetic results are explained on the basis of Ni-substitutions on octahedral sites associated with a negative contribution to the total magnetocrystalline anisotropy, thereby shifting the T at which the magnetocrystalline anisotropy constant K1 changes sign, to higher T.

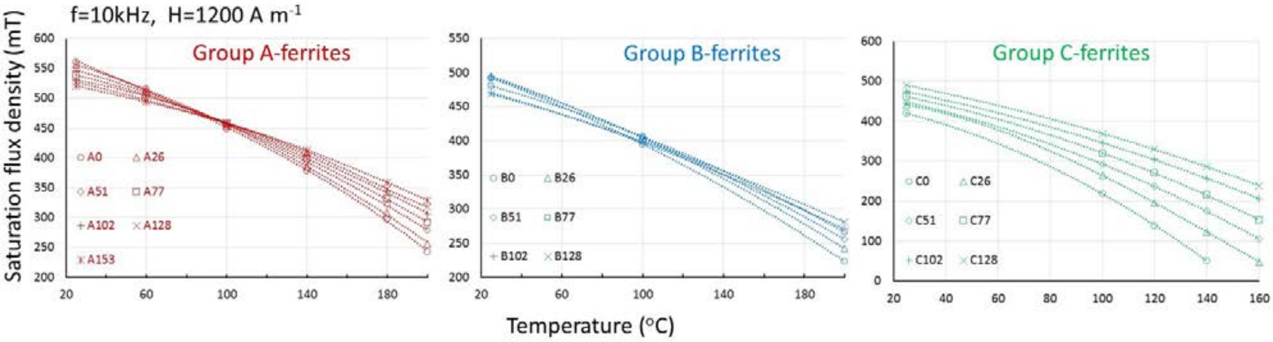


Figure 1. The saturation flux density as a function of temperature and Ni content in ferrites of Groups A, B, C.

Noncollinear magnetism and transport properties in MnPtGa films

A.Markou[1,2], E. Lesne[1], R. Ibarra[1], B. Ouladdiaf[3], K. Beauvois[3], B. Sabir[4], J. Gayles[4], C. Felser[1]
[1]*Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany*
[2]*Physics Department, University of Ioannina, 45110 Ioannina, Greece*
[3]*Institut Laue-Langevin, 6 rue Jules Horowitz, BP 156, Grenoble Cedex 9 F-38042, France*
[4]*Department of Physics, University of South Florida, Tampa, FL 33620, USA*

Abstract

Magnetic materials hosting noncollinear magnetic order have gained significant attention in the fields of condensed matter physics and material science due to their potential for future spintronic applications. One such magnetic material is the centrosymmetric hexagonal Heusler compound MnPtGa.

In this work, we present the structural, magnetic, and transport properties of hexagonal MnPtGa epitaxial thin films. We found that these films show perpendicular magnetic anisotropy. Below a thermally induced spin reorientation transition at 160 K, the magnetic ground state, determined by single-crystal neutron diffraction, is a noncollinear spin-canted state where the Mn moments tilt 20° away from the *c* crystallographic axis [1].

In addition, we observed a strongly nonmonotonic behavior in the anomalous Hall conductivity (AHC) of MnPtGa epitaxial films as a function of temperature, with the AHC changing sign at T* = 110 K across all investigated film thicknesses (20-60 nm). This suggests a common intrinsic mechanism governing both the sign and magnitude of the anomalous Hall effect (AHE). Our findings, along with first-principle calculations, strongly indicate an AHE of intrinsic origin, driven by a momentum-space Berry curvature mechanism [2].

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Synthesis and characterization of magnetic nanoparticles from rare earth – transition metal

E. Dedousi, A. Makridis, C. Sarafidis
School of Physics, Aristotle University of Thessaloniki, Greece

Abstract: Sm-Co is a well-known system which includes some compounds with excellent magnetic properties like $SmCo_5$, making it useful in a plethora of applications, especially in bulk permanent magnets. Its potential is extended also in the nanoscale where magnetic nanocomposites are gaining advantage in new, advanced technological fields. The main concern of this work is the synthesis and characterization of Sm-Co magnetic nanoparticles (NPs) produced by bottom-up methods. Following a new, simplified chemical synthesis, we explored whether this process is, in both terms of the availability of raw materials, as well as the ease of setting up the necessary devices and instruments, easier to conduct. More specifically, using samarium and cobalt nitrides as precursors, we conducted a synthetic process via two-stage heating, first stage being at 726 ^{o}C for 12h, and second stage at 560 ^{o}C for 12h. Both temperatures can be easily achieved by a common lab oven. The prepared precursor powder was then mixed with Ca, KCl and CaO, and again heated at 1100 ^{o}C for 1.5h under an Ar atmosphere, creating the final product. After each step, the powder was washed with deionized water and centrifuged at 6000 rpm/m for 10min. A part of the final product is magnetically separated and characterized by means of X-ray diffraction and Vibrating Sample Magnetometry. Due to agglomeration of the particles, a full magnetic separation is not possible as is depicted in the X-ray diffraction patterns, however, the measurements revealed the presence of a hard magnetic phase. The combined magnetization was measured above 6 Am^2/kg, as shown in Figure 1. The results are promising, especially when compared with the yield of other methods for chemical synthesis of Sm-Co nanoparticles.

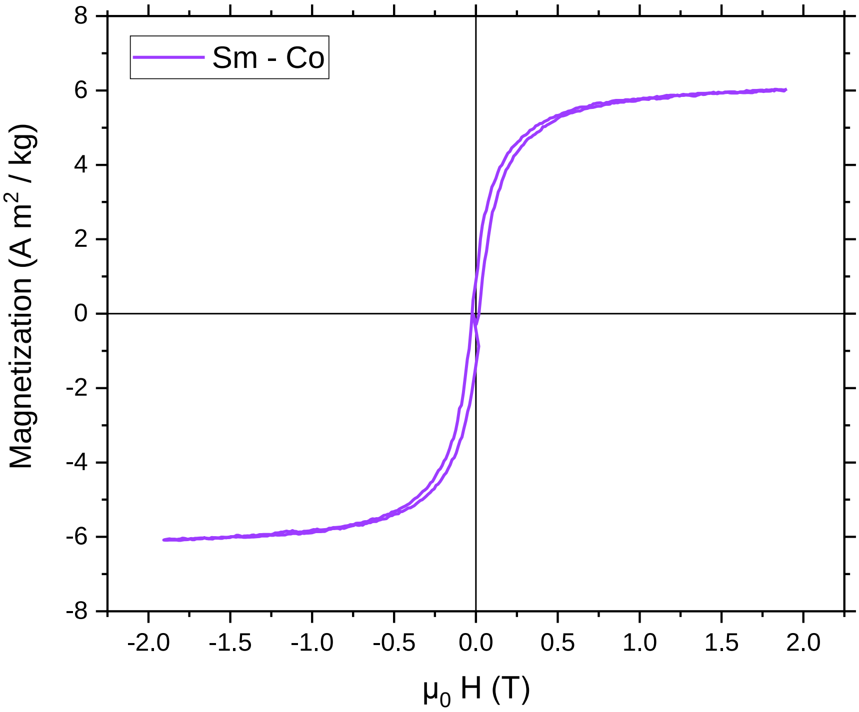

Figure 1: Hysteresis loop of the synthesized Sm-Co nanoparticles, showing their magnetic behavior and demonstrating a saturation magnetization above 6 Am^2/kg.

Studying Inter-Trap competition with a dominant last trap by simulating multi-peak Thermoluminescence Glow-Curves of wide-bandgap semiconductors

A. Touliopoulos[1], G. Kitis[1]
[1]Physics Department, Aristotle University of Thessaloniki, 54124-Thessaloniki, Greece

Abstract: Thermoluminescence (TL) is the light emission by heating semiconductors and insulators, previously irradiated by ionizing radiation (photons, electrons, neutrons, ions). The TL peaks originate from the de-excitation of electron–hole trap pairs within the forbidden band. This effect finds a wide range of applications particularly in radiation dosimetry, and requires that the radiation dose and the number of trapped electrons are correlated. The correlation is strongly affected by competition between electron traps, which impacts the trapping of electrons freed from the conduction band during irradiation and heating. In the present work, the competition between four electron traps responsible for specific TL peaks from one recombination center is simulated, with the aim of producing experimentally verifiable results. Experimental verification requires that during heating trapped electrons must be released into the conduction band within a temperature limit of 500ºC. This requirement is only met in materials whose energy band gap is smaller than 4 eV. The simulated system produced a TL glow curve consisting of four individual TL peaks as a function of trap occupancy (radiation dose) under six different competition conditions. The system was chosen so the first three TL peaks are subject to competition by the forth TL peak, which becomes the competitor and grows independently. The individual parameter values of all traps were evaluated by analyzing the simulated TL glow curves via computerized glow-curve deconvolution (CGCD) analysis. Under strong competition the TL dose response of peaks 1, 2 and 3 showcased consistent non linear behavior whereas the TL peak 4 presented the characteristics of a single trap phenomenological model, similarly the activation energy of each trap remained largely unaffected. Finally, we propose potential experiments on materials with an energy band gap smaller than 4eV in order to verify the validity of our phenomenological model.

Structure and dynamics of Hydroquinone by means of Ultrasonic Relaxation Spectroscopy, Vibrational Spectroscopy and Theoretical Calculations

A. Tryfon[1], A.G. Kalampounias[1, 2]
[1]Department of Chemistry, University of Ioannina, GR-45110 Ioannina, Greece
[2]University Research Center of Ioannina (URCI), Institute of Materials Science and Computing, GR-45110 Ioannina, Greece

Abstract: It is presented a comprehensive study of the structure and dynamics of Hydroquinone (HQ) by combining ultrasonic relaxation spectroscopy, vibrational (Raman and IR) spectroscopies, and theoretical calculations. In an effort to elucidate the underlying mechanisms that take place in the structure of the system, both ultrasound absorption and velocity have been measured and analyzed. Acoustic spectra revealed two distinct Debye-type relaxation processes occurring in the solutions, which are attributed to the self-aggregation of HQ and the protonation reaction. The formation of HQ aggregates was established by means of molecular docking calculations and the so obtained structures of the aggregates were further used to calculate the theoretical Raman and IR spectra via Density Functional Theory (DFT) calculations. The structures of the protonated species were also studied theoretically by DFT methodologies. To complement these findings, FT-IR and Raman vibrational spectra were compared with the corresponding theoretical spectra, providing additional insights into the molecular interactions. Furthermore, supplementary measurements of several physical properties, such as mass density, shear viscosity, sound speed and pH, were performed and it was confirmed that the self-association of HQ occurs mainly in the high-concentration region. The combined use of acoustic spectroscopy with theoretical calculations permitted to disentangle the underlying structural mechanisms and evaluate the volume changes associated with each mechanism. The results were compared with the corresponding theoretically predicted volume changes and discussed in the context of the concentration effect of intermolecular bonding. The research extended to assess the chemical reactivity and biological activity of both HQ monomers and dimers, considering their tendency to form aggregates in aqueous environments and in the solid state. This multifaceted analysis, not only provide a deeper understanding of the molecular behavior of HQ in aqueous solutions, but also offered valuable insight into its potential chemical and biological interactions.

Synthesis and characterization of the inclusion complex β-CD/BPE by means of vibrational spectroscopy, DSC and theoretical calculations.

I.P. Georgoulas[1], A. Tryfon[1], C. Kouderis[1], A.G. Kalampounias[1, 2]
[1]*Department of Chemistry, University of Ioannina, GR-45110 Ioannina, Greece*
[2]*University Research Center of Ioannina (URCI), Institute of Materials Science and Computing, GR-45110 Ioannina, Greece*

Abstract: It is presented the investigation of the complexation mechanism between β-cyclodextrin (β-CD) and trans-1,2-Bis(4-pyridyl) ethylene (BPE). To elucidate the inclusion process, a combination of vibrational spectroscopies (Raman and IR), Differential Scanning Calorimetry (DSC), and theoretical calculations were utilized. Molecular docking calculations theoretically confirmed the formation of the β-CD/BPE complex, revealing that BPE is encapsulated within the hydrophobic cavity of β-CD via host-guest noncovalent interactions. Molecular docking in conjunction with Density Functional Theory (DFT) provided a thorough investigation of the system and the molecular interactions involved. The interactions between the two molecules were found to be primarily driven by hydrogen bonding and Van der Waals interactions. To complement these findings, the experimental FT-IR and Raman spectra were recorded that confirmed the formation of the inclusion complex. A direct comparison with the corresponding theoretical spectra was implemented to corroborate the experimental results. The FT-IR spectra unveiled interactions between β-CD and BPE, while Raman spectra provided additional insights into the complexation mechanism. To further clarify the formation of the complex, Differential Scanning Calorimetry (DSC) was conducted in a quantitative way. The thermal analysis revealed a significant change in the thermal behavior of BPE when complexed with β-CD. The combined use of IR, Raman, DSC, and theoretical calculations provided a comprehensive understanding of the inclusion process, offering a detailed view of the molecular interactions and structural changes involved in the complexation of β-CD with BPE.

Structural Study of Salicyl Hydroxamic Acid and its Inclusion Complex with β-Cyclodextrin by Means of Vibrational and Ultrasonic Relaxation Spectroscopies, DSC and Theoretical Calculations

D. Apostolidou[1], D. Theodoropoulou[1], A. Tryfon[1], C. Kouderis[1], A.G. Kalampounias[1, 2]
[1]*Department of Chemistry, University of Ioannina, GR-45110 Ioannina, Greece*
[2]*University Research Center of Ioannina (URCI), Institute of Materials Science and Computing, GR-45110, Ioannina, Greece*

Abstract: In this work, we present a comprehensive analysis of the structure of Salicyl Hydroxamic Acid (SHA) and the mechanism behind its inclusion complex formation with *β*-cyclodextrin (*β*-CD). Several experimental techniques including ultrasonic relaxation spectroscopy, vibrational spectroscopies (IR and Raman), Differential Scanning Calorimetry (DSC), and theoretical calculations were utilized. The structural changes in SHA were elucidated by ultrasound absorption measurements. Two distinct Debye-type relaxation processes were identified in the acoustic spectra that are attributed to the self-aggregation of SHA and to the proton transfer reaction. Molecular docking calculations revealed the formation of SHA aggregates. The so obtained structures of the aggregates were further used to compute theoretical Raman and IR spectra using Density Functional Theory (DFT). Except aggregate species (dimers), monomer and the protonated species were also studied theoretically using DFT methodologies. To elucidate the mechanisms behind these findings, theoretical and experimental IR and Raman spectra were compared. Additional measurements of mass density, shear viscosity, and pH were performed to validate the aggregation and proton transfer mechanisms within the molecule, demonstrating that SHA self-association occurs mainly in the high-concentration region. Molecular docking calculations further established the formation mechanism of the inclusion complex, confirming the presence of a hydrogen bond between SHA anf *β*-CD. The experimental study of the system involved obtaining the *β*-CD/SHA complex in the solid state by means of the Drop Casting method. The experimental Raman and IR spectra of the solid were compared with the calculated theoretical spectra. These results were supported by DSC method, which revealed a significant change in the thermal behavior of the inclusion complex. These results established the encapsulation of the SHA into *β*-CD cavity. This comprehensive analysis not only provides a deeper understanding of the structural properties of SHA, but also offers valuable insights into its potential application in drug delivery systems.

(Hyper)Polarization Effects in Molecular Materials

Aggelos Avramopoulos[1,2], **Eırını Faropoulou** [1,2],
[1]*Department of Physics, University of Thessaly, Lamia, Greece;* [2] *Postgraduate Course Program: "Applied Physics", Department of Physics, University of Thessaly, Lamia, Greece*

Abstract: *Design at the molecular level* is an important issue for material science. One specific challenge is the understanding of factors that govern light-matter interactions and how one can tune them in an efficient way. The Linear and Non-Linear (L&NLO) properties are of great current interest, because they allow to advance our understanding of the electronic and vibrational structure of the molecules. In addition, they are key parameters for the design of materials with many applications (e.g., fiber optic communication, all optical switching)

A series of molecular materials with exceptional high NLO properties were computationally designed with the aid of Density Functional Theory (DFT) (spin-broken wavefunction). These include Fig. 1: **I)** 1D and 2D coordination polymers (nanosheets), based on nickel bis(dithiolene) and benzene (), **II)** Oligomer of (RA-NiBDT)**n**, RA = radiaannulene, **III)** Polycyclic Aromatic Hydrocarbons (PAH) (0D graphene quantum dots). Main objective was to demonstrate the superior non-linear optical (NLO) performance of the proposed materials, which involved NiBDT (bis(ethylene-1,2-dithiolato)Ni,), fused with a series of rich p-electron organic linkers:

The following key points were found: **1.)** Great dependence of the polarizability and second, electronic and vibrational hyperpolarizability, with the linker which the NiBDT units are fused, **2)** Enhancement of the NLO character is achieved by involving a series of units of NiBDT, π-electron rich linker, metal atoms (e.g Li), **3)** 1D arrangement appears to have a much larger second order hyperpolarization in comparison to the corresponding 2D one (γ(3)/γ(2) = 23.9), attributing to the much larger diradical character of 3, **4)** Global Hardness in PAHs, which is a measure of the inhibition of charge transfer and associated with the polarization character, depends on the size, shape and edge of the considered PAH.

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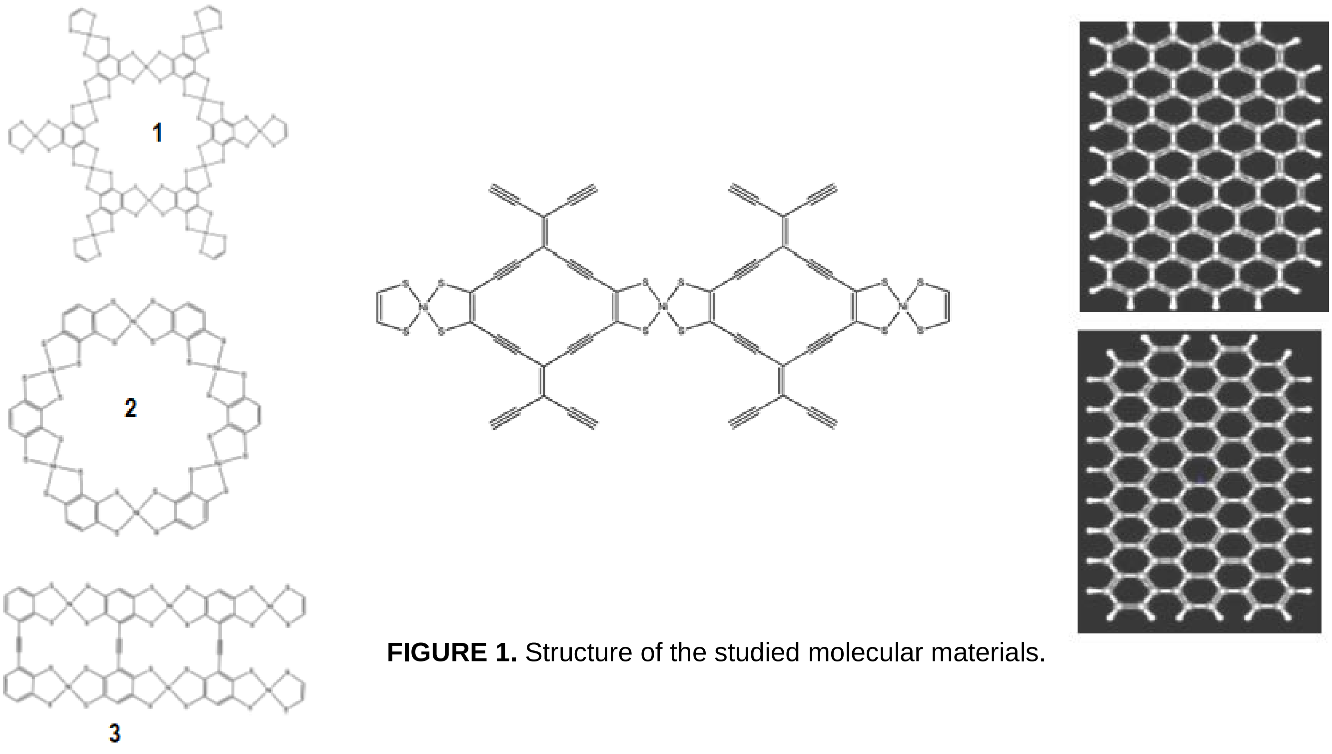

FIGURE 1. Structure of the studied molecular materials.

Symbolic machine learning expressions for fluid properties in nanochannels

Ch. Georgakopoulos[1], D. Angelis[1], F. Sofos[1], T.E. Karakasidis[1]
[1]Condensed Matter Physics Laboratory, Department of Physics, University of Thessaly, Lamia, Greece

Abstract:

The calculation of fluid transport properties in nano-confined devices is important both for theoretical understanding and applications. Fluid properties alter significantly under confinement and well-established numerical simulation models, such as molecular dynamics, have proven to be invaluable for their investigation. Nonetheless, the computational burden associated with that kind of models makes this approach resource and time demanding. The advent of data-driven models has mitigated some of these challenges by enabling fast predictions without sacrificing accuracy. However, most of these models suffer from interpretability issues due to their “black-box” nature and they cannot infer physical explanation to the result, which would make them generalizable. We propose an alternative road that not only utilizes the power of machine learning approaches but can also express the dynamics with respect to system parameters. Symbolic regression, a regression-based machine learning method, is exploited to model a quantity of interest as a function of system variables, while concurrently adhering to physical limitations, without the need to incorporate prior knowledge [1]. Here, we present results for the diffusion coefficient of various molecular fluids under confinement [2] and suggest symbolic expressions that accurately describe the phenomenon. These expressions are general, depend on the system parameters, and can provide the diffusion coefficient values in a wide range of the input parameter space. This procedure can be used in parallel to classical numerical simulation methods, which are important to calibrate and validate the result. Overall, we propose a transparent linkage between the system parameters and the result, offering a new, alternative perspective on computational approaches and ways to accelerate the construction of nano-confined systems.

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Acknowledgement

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Fe_3O_4 magnetic nanoparticles coated with amorphous mSi-Ca shell for encapsulation of pharmaceutical substances

D. Kordonidou[1], G. K. Pouroutzidou[2,3], I. Tsamesidis[2,3], K. Kazeli[4,5], K. Tsachouridis[6], A. Anastasiou[6], G. Vourlias[1,2], M. Angelakeris[4,5], E. Kontonasaki[3]
[1]Department of Physics, Aristotle University of Thessaloniki, Greece
[2]Laboratory of Advanced Materials and Devices, Department of Physics, Aristotle University of Thessaloniki, Greece
[3]Division of Prosthodontics, Department of Dentistry, School of Health Sciences, Aristotle University of Thessaloniki, Greece
[4]Department of Condensed Matter and Materials Physics, AUTh, Thessaloniki, 54124, Greece
[5] Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Thessaloniki, 57001, Greece
[6]Departmentof Chemical Engineering, the University of Manchester, Oxford Rd, Manchester M13 9PL, United Kingdom

Abstract:

The present work concerns the synthesis of magnetic core-shell nanoparticles (NPs) of magnetite (Fe_3O_4), coated with Ca-doped SiO_2 shell. For core's synthesis (Fe_3O_4 NPs), aqueous solutions of $FeCl_3$ and $FeSO_4$ were mixed(1) within a three-necked flask. The mixture was then subjected to heating at 60°C, under an Ar atmosphere, with simultaneous magnetic stirring. Ammonia solution was added to the aqueous solution, which was stirred with glycerol-controlled argon flow (pH=10). After washing with deionized, the solution was subjected to centrifugation and drying afterwards overnight at 75°C.

Regarding the mesoporous shell enriched with Ca ions' synthesis around the magnetic NPs (Fe_3O_4/mSi/Ca NPs), an aqueous solution of Fe_3O_4 was subjected to ultrasonic dispersion with a probe sonicator. Ethanol, CTAB, and NH_3 were added to the solution(2), which was once more subjected to stirring and probe sonication. A drop-by-drop addition of TEOS followed, the solution was then stirred for 2h (1st sample) and 30' (2nd sample). Afterwards, $Ca(NO_3)_2{\cdot}4H_2O$ was added and the solution was stirred anew at 37°C for 15 hours, washed with ethanol, dried overnight at 60°C and then put to calcination for 2h at 350°C. The results revealed an approximately spherical shape for most particles, small size distribution and slight agglomeration. Particles were crystalline with mean size ~13nm and were successfully coated with a Ca/SiO_2 shell. NPs also presented diffraction peaks similar to face-centered cubic crystal structure of Fe_3O_4, although, a cubic crystal structure of Fe_2O_3 was also detected. A mild core toxicity and good biocompatibility for the shelled NPs was confirmed via MTT analysis. Future research includes: evaluation of NPs magnetic properties, investigation of in vitro development of biological hydroxyapatite, study of the induction of osteogenic differentiation of mesenchymal stem cells and encapsulation of pharmaceuticals and biological molecules to accomplish their controlled release under an appropriate magnetic field.

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Thermal exfoliation as a prominent green method for increasing the photocatalytic performance of g-C_3N_4 prepared from different precursors

C. Lykos[1], A. Triptsi[1], E. Karypidou[1], I. Konstantinou[1,2]
[1]*Department of Chemistry, University of Ioannina, Ioannina 451 10, Greece*
[2] *Institute of Environment and Sustainable Development, University Research and Innovation Center of Ioannina, 45110 Ioannina, Greece*

Abstract: In the past two decades, heterogeneous photocatalysis gained significant ground in the fields of green energy production and wastewater remediation. According to the existing literature, TiO_2 has been extensively utilized as a photocatalyst in various applications. However, the fact that it can be photoactivated only under UV radiation, harnessing about ~ 4% of solar energy, severely limits its applicability as a solar photocatalyst. In this light, many studies have focused on the synthesis and application of visible light-activated (VLA) photocatalytic materials that can utilize more photons of the solar spectrum. Among the various VLA photocatalysts developed, the emerging graphitic carbon nitride (g-C_3N_4) has demonstrated many attractive characteristics such as non-toxicity, stability in a broad pH range, chemical stability and more. Despite all these features, a key drawback of bulk g-C_3N_4 is the high recombination rate of the photogenerated charges that decreases its photocatalytic performance. To date, many different approaches have been proposed for enhancing the efficiency of g-C_3N_4, but most of these methods require further complex synthetic steps and the use of expensive chemicals, increasing production costs. According to a few studies, a low-cost facile approach to improve g-C_3N_4 is to thermally exfoliate its stacked 2D layers. In view of this, the present work investigated the effect of thermal exfoliation of urea and thiourea-derived g-C_3N_4 by subjecting them to three thermal treatment cycles. The structure, composition and optical characteristics of the synthesized materials were studied through various techniques (XRD, FESEM, EDS, ATR-FTIR, Raman, DLS, DRS and Photoluminescence spectroscopy). Additionally, their photocatalytic performance was evaluated by conducting lab-scale experiments using a sunlight simulator. The insecticide Clothianidin was chosen as a model pollutant, and the results revealed that the thermally exfoliated materials are much more efficient photocatalysts compared to their bulk counterparts.

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High-resolution laser digital transfer of Graphene

K. Magoula[1], K. Andritsos[1], F. Zacharatos[1], C. Katopodis[1], A. Zurutuza[2], A. Centeno[2], A. Rebollo[2], Y. Papadopolos[1], L. Tsetseris[1] and I. Zergioti[1]

1. Department of Physics, School of Applied Mathematical and Physical Sciences, National Technical University of Athens, 15780 Athens, Greece.
2. Graphenea Headquarters, Paseo Mikeletegi 83, 20009 - San Sebastián, Spain

Interest for the use of two dimensional (2D) materials (especially graphene) in electronics and optoelectronics has grown steadily over the last several years, driven by their unique structure-related properties which set them apart from bulk materials of similar composition. By the same token, however, there are key open issues in this field which need to be addressed, in order for pertinent basic research efforts to mature into widely used technologies. One of these challenges is the precise and controllable transfer of graphene and other 2D materials from their growth substrate to a target wafer. In this work, we use an advanced laser technique to achieve the non-defective, maskless, and polymer-free digital transfer of graphene. We present results on the deposition of graphene pixels onto SiO_2(300nm)/Si substrates, with spot sizes ranging from 10 μm to 50 μm. The method employs a telecentric 4f optical system with an infinity-corrected long working distance microscope objective lens and a plano-convex lens, while the shape and size were adjusted using a variable aperture square mask. The transferred graphene pixels were examined with optical microscopy, Scanning Electron Microscopy (SEM), and Raman spectroscopy measurements. These characterizations verified that high-quality monolayers of graphene were deposited, while electrical characterization has confirmed that the transferred graphene pixels retained their outstanding foundry values of high carrier mobility and low electrical resistivity. The good control on the size and shape of the deposited graphene specimens enables their incorporation within photonic integrated circuits, of on-chip photodetectors and modulators, on top of Au electrodes and SiN waveguides, with a maximum step height of 33 nm.

Unveiling superlubricity in 2D heterostructures: Tailored forcefields driven by precision DFT calculations

G. Fanourgakis[1], C.S. Garoufalis[2], E. Papasouli[1], C. Androulidakis[3,4], E.N. Koukaras[1]
[1]Laboratory of Quantum and Computational Chemistry, Aristotle University of Thessaloniki, Thessaloniki, 54124, Greece
[2]Materials Science Department, University of Patras, 26504 Patras, Greece
[3]Prometheus Division of Skeletal Tissue Engineering, KU Leuven, O&N1, Herestraat 49, PB 813, 3000 Leuven, Belgium
[4]Skeletal Biology and Engineering Research, KU Leuven, ON1 Herestraat 49, PB 813, 3000 Leuven, Belgium

Abstract: In this study, we investigate the superlubric behavior of two-dimensional (2D) heterostructures through an advanced combination of established computational techniques. We develop an *ad hoc* tailored forcefield to accurately model and optimize the frictional properties of these materials. The parameterization of the forcefield is based on results of high-accuracy density functional theory (DFT) calculations with non-local treatment of dispersion interactions, ensuring precise representation of atomic interactions and frictional forces.

Our research examines conditions that trigger the potential of 2D heterostructures to exhibit superlubricity, a phenomenon where friction is significantly reduced or nearly eliminated at the interface of sliding layers. By employing the newly developed forcefields, we can simulate and predict the behavior of these materials under various conditions.

The results of our simulations reveal the critical parameters and conditions necessary to achieve superlubricity in 2D heterostructures. Our findings not only contribute to the fundamental understanding of friction at the nanoscale but also provide essential insights for designing materials with enhanced tribological performance and their potential applications in nanotechnology and material science. This work also highlights the crucial combination of high-accuracy first-principles calculations and tailored computational models in exploring and optimizing the unique properties of 2D heterostructure materials.

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). CA acknowledges support by the Research Foundation Flanders (FWO) through the grants 1260722N and V478123N. 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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INFLUENCE OF SURFACE STRUCTURE ON FURFURAL CONVERSION: COMPARATIVE STUDIES ON Ni(111) AND NiO(111) SINGLE CRYSTAL SURFACES

A. K. Bikogiannakis[1], F. Xydas[1], A. S. Stylla[1], S. Tsatsos[1] and G. Kyriakou[1]
[1]*Department of Chemical Engineering, University of Patras, Karatheodory 1, Rion, Greece*

Abstract:

The interaction of organic molecules with metal and metal oxide surfaces is of profound importance in a large number of technological applications including heterogeneous catalysis, organic electronics and advanced functional materials. In regard to heterogeneous catalysis, adsorption and reactivity studies of organic molecules on single crystal surfaces can facilitate our understanding of how reaction mechanisms proceed. Highly functional organic molecules, like furfural, are of great interest in such applications, as they act as 'platform' compounds, from which a number of useful chemicals and chemical intermediates can be produced, with the power to transform global energy and materials markets. The hydrogenation of furfural has already been studied on monometallic platinum[1] and copper[2] dispersed catalysts, PtCu and PdCu bimetallic catalysts, ultra dilute and single atom alloys.[3–5] Our work has been extended to the use of model catalytic single crystal surfaces, which allow the study of the surface reactions by focusing on the electronic and geometric interactions of the adsorbed molecules with the surface.[6,7] Here, we have studied the adsorption and reactivity of furfural on Ni(111) and NiO(111) single crystal surfaces under Ultra High Vacuum (UHV) conditions, employing Temperature Programmed Desorption/Reaction and X-Ray Photoelectron Spectroscopy. Our findings reveal that pristine Ni(111) selectively favors propene formation from furfural, suggesting a pathway involving hydrogenation and subsequent carbon-carbon bond cleavage facilitated. In contrast, pristine NiO(111) exhibits negligible reactivity towards furfural, with only furan traces produced, through the decarbonylation pathway. Interestingly, even slightly doping the surface with oxygen passivates 2-methylfuran production, stating the inhibition of the hydrodeoxygenation pathway. These insights into the surface-dependent catalytic behavior of nickel surfaces provide valuable guidelines for designing more effective catalysts for furfural conversion to promising biofuels. They underscore the importance of surface composition and structure in determining catalytic performance, with potential implications for industrial applications in sustainable chemistry.

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Towards Quasiparticle Poisoning Rates of Quantum Dots in an InAs/Al Hybrid Heterostructure

V. Vlachodimitropoulos[1], A. Author[2], A. Author[3], …
[1]*Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark*

Abstract:

Superconductor-semiconductor (SC-SM) hybrid devices hold great promise for the development of topological states of matter that can demonstrate non-Abelian statistics and potentially be used as a platform for topologically protected quantum computing. Despite significant theoretical and experimental efforts, the unequivocal demonstration of such states remains elusive. However, recently it was shown that a weakly-protected version of these states could be experimentally realised in SC-SM hybrid systems. These weakly protected states appeared at the ends of a two-site Kitaev chain, which was physically implemented with a pair of quantum dots connected via an Andreev Bound State living in a grounded superconducting segment between them. Even in these weakly protected systems, quantum information is encoded non-locally and, as a result, they are expected to exhibit enhanced resilience to typical local noise sources. However, despite this non-local storage of information, there are still noise channels through which quantum information may be corrupted. A prominent example of such a channel is a single electron tunnelling event between a semiconducting and a superconducting region, usually referred to as quasiparticle-poisoning (QPP). In these topological systems, fermion parity is the resource that is used to store quantum information, and since QPP events may change the parity, they can thus destroy quantum information. Therefore, the QPP-free time scale is of critical importance as it determines the time in which quantum computations can be accurately performed. The goal of this project is to estimate the rate of QPP events of a system composed of a quantum dot next to a superconductor. In this work, I will discuss the design considerations for the devices that are under development in our lab to estimate QPP rates, present the first generation of devices along with the fabrication challenges that are being addressed, and show preliminary data on their performance.

Microwave Perfect Absorbers (MPAs) based on Ag-metal printed patterns

Gagaoudakis E.[1], Mantsiou E.[2], C.-P. Tsichlis[1], K. Dovelos[3], A. Paraskevopoulos[4], V. Vardakastani[3], D. Tzarouchis[3], M. Koutsoupidou[3], P. Kosmas[3], C. Spandonidis[5], F. Giannopoulos[5], A. Petsa[5] and Binas V.[1,2]
[1]*Foundation of Research and Technology - Hellas, Institute of Electronic Structure & Laser (FORTH-IESL), Heraklion Greece*
[2]*Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece*
[3]*Meta Metamaterials Europe, Ap. Pavlou 10, 15123, Marousi, Athens, Greece*
[4]*Institute of Informatics and Telecommunications, NCSR Demokritos, 15310 Athens, Greece*
[5]*Prisma Electronics SA, 87 Dimokratias Ave., 68100, Alexandroupolis, Greece*

Abstract: Metamaterials are artificial materials with unique and unusual properties based on their geometric designs. They can be used in numerous applications such as invisible cloaking, signal sensing and wave absorption. In this work, metallic patterns created using additive manufacturing (3D printing) techniques on a flexible substrate were investigated as perfect absorbers for electromagnetic waves in the region of 8 GHz to 12 GHz. Specifically, various topologies were designed, simulated, and developed to control surface impedance and achieve electromagnetic absorption at 8 GHz[i] (Fig. 1). The level of transmission and reflection of the developed samples was measured with WR137 and WR112 waveguides. Also, their surface impedance was also estimated using a method for calculating sheet impedance of thin conductive films[ii].

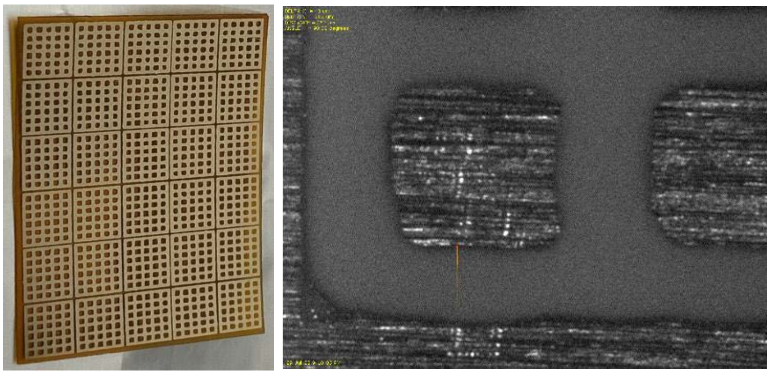

Figure 1: Printed Ag-metal pattern as Microwave Perfect Absorber (MPA)

Acknowledgements

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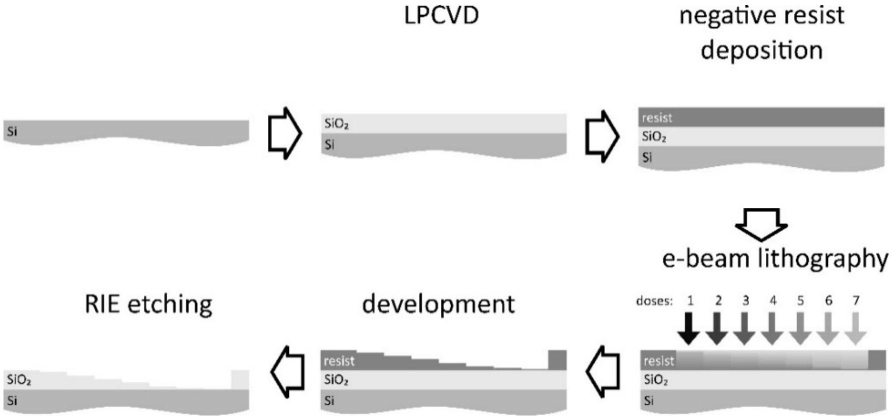
3D structured Si chip for label free determinations at the point-of-need

G.Zisis[1,2], G.Papageorgiou[1], P.Petrou[3], I.Raptis[1,2], N.Papanikolaou[2]
[1]*INN, NCSR Demokritos', Athens, Greece*
[2]*ThetaMetrisis S.A., Athens, Greece*
3INRASTES, NCSR Demokritos, Athens, Greece

Abstract:

A novel optical label-free biosensing approach is introduced aiming to remove the current limitations of optical biosensors in their application of on-site food analysis. The proposed methodology (GRADual thin film IntErferometry, GRADE) is based on light interferometry employing an illumination source of a few nm spectral width and a 3D micro-patterned sensor surface consisting of multilevel staircase structures, fabricated through grayscale electron beam lithography and appropriate pattern transfer on thick dielectric layer. The formation of the biomolecular adlayer on the 3D structured surface sensor, is monitored with a 2D camera, without the need for broadband illumination sources and spectral analysis instrumentation. Consequently, this novel sensing approach has the potential to enable the cost-efficient monitoring of bioreactions employing a simple optical setup, a low-cost photodetector and light source, thus being an ideal platform for use at the Point-of-Need. In the present study the system is demonstrated for the detection of aflatoxin B1 (AFB1), a very potent carcinogen detected in various food categories.



Schematic of the fabrication steps of the sensing area: staircase profiles of linearly changing thickness on SiO_2 layer are achieved by modulating the EBL exposure dose.

Interface defects in p-type Ge/Al_2O_3/Al capacitors

Vassilios Ioannou-Sougleridis[1], Stamatios Alafakis1, Dimitrios Skarlatos[2].
[1] *Institute of Nanoscience and Nanotechnology, National Center for Scientific Research Demokritos,Agia Paraskevi Attikis, P.O.Box 60037, 153 10 Athens, Greece,*
[2] *Department of Physics, University of Patras, 265 00 Patras, Greece*

Abstract:

High mobility semiconductors like Ge will always attract interest as an alternative channel material to that of silicon. Indeed, their higher mobility could help to improve IC CMOS performance. One of the central issues of Ge integration as a channel material is the fabrication of a high stability Ge dielectric interface with a low density of interface traps. This has been proved to be a quite difficult issue, because GeO is volatile and diffuse easily through the growing or deposited dielectric. This inherent instability of the Ge interface requires the introduction of customized techniques for the production of high-quality interface. In this work an analysis of the conductance-voltage characteristics of p-type Ge/Al_2O_3/Al capacitors as a function of temperature is presented. The analysis reveals the presence of two loss peaks in the interface trap conductance (G_{it}) vs normalized surface potential (u_s) characteristics. One loss peak is attributed to the generic interface traps that typically exists in a semiconductor-insulator interface with a distributed density across the energy gap. The second loss peak is located very close to the valence band edge (0.05 eV or less) and shows no shift with temperatures changes, a fact which suggest a bulk defect. This defect can be attributed to the reflection of the peroxy linkage defect at the Ge-Al_2O_3 interface. Both defects are suppressed significantly by post metallization annealing performed at 350 ^oC in nitrogen ambient.

Study of plasmonic effect in perovskite solar cells upon silver-nanoparticles modification of SnO_2 used as electron extraction layer

A. Soultati[1,2], G. Cahtzigiannakis[1], G. Papadimitropoulos[1,2], S. Kaminaris[2], K. Aidinis[3,4], M. Vasilopoulou[1]

[1]Institute of Nanoscience and Nanotechnology, National Center for Scientific Research Demokritos, Agia Paraskevi, 15310 Athens, Greece
[2]Department of Electrical and Electronics Engineering, University of West Attica, P. Ralli & Thivon 250, 12244, Aegaleo, Greece
[3]Department of Electrical and Computer Engineering, Ajman University, P.O. Box 346, Ajman, United Arab Emirates.
[4]Center of Medical and Bio-Allied Health Sciences Research, Ajman, United Arab Emirates

Abstract: Luminescent solar concentrators (LSCs) combined with high-efficiency, index matching opaque PV cells are an exciting solution for semi-transparent or even transparent photovoltaic glazing systems, which could potentially convert the façades of urban buildings into distributed electrical power generators hence accelerating the fabrication of efficient net-zero buildings. In this work, a highly efficient and transparent plasmon-coupled luminescent solar concentrators through the design of discrete resonator (Ag nanoparticles)-emitter core-satellite structures combined with perovskite solar cell (PSC) of high efficiency and stability is reported. In particular, silver (Ag) nanoparticles (NPs) were embedded in tin oxide (SnO_2) films used as electron transport layers in PSCs. Pristine SnO_2 and Ag-NPs SnO_2 were systematically studied regarding their properties by using cyclic voltammetry, Fourier-transform infrared (FTIR), and UV-Vis spectroscopy in order to reveal their energetic alignment and possible interaction with the perovskite layer. The localized surface plasmon resonance (LSPR) effect in the Ag-NPs SnO_2 thin film was also investigated. Comprehensive analyses, including UV–Vis absorption spectroscopy, atomic force microscopy, photoluminescence spectroscopy, and electrical measurements, confirm the synergistic core-shell influence of the encapsulated Ag NPs. Then, pristine and Ag-NPs modified SnO_2 applied as interlayers between an indium-tin oxide electron selective electrode and perovskite absorber. Optoelectronic measurements indicate that Ag-NPs SnO_2 devices present significant enhancement in performance and stability due to the LSPR effect. The application of low-cost solution-processed materials in perovskite solar cells may be attributed to their wide implementation in large area applications.

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ELECTRONIC STRUCTURE AND MODELING PROPERTIES OF PEROVSKITE A_2ZrX_6 MATERIALS, WHERE A= $(CH_3)_3S$, $CH_3NH_3^+$, $CH(NH_2)_2^+$ and X= Cl, Br, I

C. Kolokytha [1, 2], N. N. Lathiotakis [2], D. Tzeli [1, 2]

[1] Laboratory of Physical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Zografou, GR-15784, Greece

[2] Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens, GR-11635, Greece

Perovskites is a versatile class of compounds of the general composition ABX_3, where A and B are two cations with different sizes from each other and X is an anion. Nowadays, halide perovskites that contain lead have applications in microelectronics, solar sell systems, laser crystals, light-emitting diodes-LEDs, photoelectrolysis, etc. [1].

In the present research, novel compounds with the tetravalent metal Zr are studied, where the A groups are $(CH_3)_3S$, $CH_3NH_3^+$, $CH(NH_2)_2^+$ and X groups are halogens such as Cl, Br, I. Note, that this class of materials forms 0D crystal structures with isolated $[ZrX_6]^{2-}$ octahedra and is known as defect perovskites (also known as K_2PtCl_6 structure type) with lower toxicity and higher stability in air than lead perovskites.

The A_2ZrX_6 materials are calculated employing the Density Functional Theory using the GGA/PBE, hybrid (HSEsol, HSE06) and Meta-GGA (MBJ) functionals for periodic calculations on finite structures. The aim is to determine the optimized crystal structure and their electronic properties.

The results of the computational study showed that the band gap is affected by the choice of the used functionals. The best ones are the hybrid (HSE06) and Meta-GGA (MBJ) functionals which predict the band gap energy of the $[(CH_3)_3S]_2ZrCl_6$ material in agreement with the corresponding experimental value [2]. Moreover, from the Density of State (DOS) and Band Structure plots, it is found that the change in band gap energy is affected by both the halogen anion and the A position. In particular, the decrease in halogen's magnetization (Cl>Br>I) and the increase in atomic radius (Cl<Br<I), results in a decrease in band gap energy. Finally, the change of the substituent A, affects the geometry of the material (cubic or triclinic), the size of the unit cell, the distances between halogens in the same octahedron or between different octahedra.

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Pillared Graphene Frameworks for greenhouse gases adsorption and separation

E. Papasouli[1], E. Klontzas[2], I. Skarmoutsos[3], G. Fanourgakis[1], E. Koukaras[1]
[1]Laboratory of Quantum and Computational Chemistry, Aristotle University of Thessaloniki, Thessaloniki, 54124, Greece
[2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, GR-116 35 Athens, Greece
[3]Laboratory of Physical Chemistry, University of Ioannina, Ioannina, 45110, Greece

Abstract: Pillared Graphene Frameworks (PGFs) are a novel class of materials that blend the properties of graphene for diverse applications, including transistors, optoelectronics, supercapacitors, and membranes for gas storage and separation. In this computational study, we have designed PGFs with graphene layers interconnected by various organic molecules through the formation of triazole rings. The interlayer distance of the graphene layers can be therefore precisely tuned by utilizing organic molecules of different sizes, enabling the creation of three-dimensional frameworks with adjustable pore sizes. These tunable 3D structures are particularly effective as membranes and bulk materials for gas storage and separation. In this study we investigate the storage and separation in PGFs for some common greenhouse and other gases that are important in industrial applications. Specifically, we conducted Monte Carlo simulations in the grand canonical ensemble on 3D PGF models to investigate the adsorption isotherms of pure gases such as SF_6, CF_4, N_2O and N_2. We assessed the potential of these frameworks to separate gas mixtures, focusing on SF_6/N_2 and CF_4/N_2, since N_2 is the predominant gas mixed with CF_4 and SF_6 in industrial flue gases. Our findings indicate that PGFs are promising materials for efficient gas adsorption and separation, with potential implications for environmental and industrial applications.

Acknowledgments: Results presented in this work have been produced using the Aristotle University of Thessaloniki (AUTh) High Performance Computing Infrastructure and Resources.

Work Function of Caesiated Molybdenum Surfaces under Different Water Vapor Pressures and Surface Temperatures

N. Klose[1,2], A. Heiler[2], D. Vlachos[3], R. Friedl[1] and U. Fantz[1,2]
[1] *AG Experimentelle Plasmaphysik, University of Augsburg, 86135 Augsburg, Germany*
[2] *Max Planck Institute for Plasma Physics, Boltzmannstr. 2, 85748 Garching, Germany*
[3] *Department of Physics, University of Ioannina, GR-451 10, Ioannina, Greece*

Low work function (WF) coatings are essential for versatile applications, e.g. electron emission devices, photocathodes, or negative hydrogen ion sources for accelerators and neutral beam injection (NBI) systems for nuclear fusion. For the latter case, low WF surfaces are typically created by evaporating Cs on a converter surface. Recent research has shown that under moderate vacuum conditions (10^{-7}−10^{-6} mbar) a WF of 1.2-1.5 eV is given. This WF is below the value of bulk Cs (2.0−2.1 eV) and even below the typical sub-monolayer minimum of 1.5-1.6 eV. It is assumed that the formation of Cs oxides from reactions with oxygen or/and residual water leads to this low WF values. Water is inevitably present due to the given non-ultra-high vacuum (UHV) conditions. For the international fusion experiment ITER an NBI ion source with pressure conditions down to 10^{-8} mbar is foreseen. This arises the question if such low background pressures influence the formation of Cs oxides and thereby the formation of surfaces with a WF below 1.5 eV.

To investigate the WF behaviour upon Cs and water co-adsorption, a polycrystalline molybdenum surface is caesiated in a UHV experiment, which provides the possibility to add water vapour in a controlled manner. The WF is measured absolutely via the photoelectric effect and the Fowler formalism. Up to a water pressure of 10^{-9} mbar the typical WF minimum curve is measured, with a minimum WF of 1.5±0.1 eV and an increase up to 1.9±0.1 eV for longer caesiation times. For higher water pressures, the WF decreases further and stabilizes at 1.1±0.1 eV, indicating the formation of a Cs oxide layer with a sufficient flux ratio of Cs to water onto the surface. Additionally, the effect of elevated surface temperatures up to 400°C on the WF is investigated.

Synthesis and characterization of electric double layer capacitors (EDLC) using different carbon-based nanomaterials

Lydia Gialama[1,2], Dionysis S. Karousos[1], George Theodorakopoulos[1], Fotios K. Katsaros[1],
Evangelos P. Favvas[1], Mirtat Bouroushian[2]

[1]Institute of Nanoscience and Nanotechnology, National Center for Scientific Research "Demokritos", Aghia Paraskevi, 15341 Athens, Greece
[2]School of Chemical Engineering, National Technical University of Athens, Zografou Campus, 9 Iroon Polytechniou St., Zografou Campus, 15772 Athens, Greece

Abstract:

Electric Double-Layer Capacitors (EDLC) in the form of coin cells were prepared using different carbon nanomaterials and analyzed by electrochemical techniques. In specific, water-dispersible Graphene Nano-Platelets (GNP) and Carbon Nano-Tube (CNT) materials were combined with polyvinyl alcohol (PVA) to create dry gels, which were then carbonized to produce carbon aerogels for use in EDLC electrodes. A series of different active carbon materials were prepared and combined with carbon black and polyvinylidene fluoride (PVDF) binder to form a paste (mass ratio 8:1:1), which was applied onto conductive aluminium foil, serving as back-contact, and solidified through phase inversion. In effect, the use of oxidized GNP as a precursor in double-layered or mixed active material samples resulted in the formation of stable pastes and films, having strong adhesion on aluminium contact. Variously combined double-layer and mixed active material samples were used to prepare electrodes for symmetric coin cells, which were tested as for their electrochemical properties by means of galvanic charge-discharge cycling and cyclic voltammetry (CV) measurements. Best samples demonstrated a specific capacitance of 88 F/g at charging/discharging experiments with constant 39 mA/g current density. The vast variety of possible active material combinations that can be examined in future work, based on this study, may offer insights into the development of enhanced EDLCs with improved electrochemical properties, highlighting the potential of carbon nanomaterials in energy storage technologies.

Acknowledgments

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Photocatalytic performance of $ZnIn_2S_4$/CdS hybrids for enhanced organic dye degradation and hydrogen peroxide evolution under visible light

N. Karamoschos[1], A. Katsamitros[1], D. Tasis[1,2], …
[1]*Department of Chemistry, University of Ioannina, 45110 Ioannina, Greece*
[2]*University Research Center of Ioannina (URCI), Institute of Materials Science and Computing,45110 Ioannina, Greece*

Abstract: This study explores the synthesis and application of $ZnIn_2S_4$ and CdS hybrids for the dual functions of organic dye degradation and hydrogen peroxide (H_2O_2) evolution. These semiconductor materials were selected for their promising photocatalytic properties under visible light irradiation, a crucial factor for sustainable energy-related applications. The $ZnIn_2S_4$/CdS hybrids were synthesized using a hydrothermal method, resulting in well-defined, crystalline structures with enhanced surface areas. Characterization techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), confirmed the successful formation of the hybrid materials and their desirable optical properties.

Photocatalytic performance was evaluated by degrading Orange G a common organic dye, under visible light. The results demonstrated significantly higher degradation rates for the $ZnIn_2S_4$/CdS hybrids compared to the individual components, attributed to efficient charge separation and extended light absorption range. The degradation kinetics followed a pseudo-first-order model, with rate constants markedly improved over pure $ZnIn_2S_4$ and CdS.

Additionally, the hybrids' ability to produce hydrogen peroxide under visible light was investigated. The experiments revealed that the $ZnIn_2S_4$/CdS hybrids not only facilitated higher H_2O_2 generation rates but also maintained stability and reusability over multiple cycles. This enhanced performance is likely due to the synergistic effects between $ZnIn_2S_4$ and CdS, which promote efficient electron-hole separation and reduce recombination rates.

The study concludes that $ZnIn_2S_4$/CdS hybrids are promising candidates for photocatalytic applications. Their dual functionality in dye degradation and H_2O_2 evolution under visible light conditions underscores their potential as multifunctional materials for sustainable technological advancements. Future work will focus on optimizing synthesis parameters and exploring real-world applications to further validate these findings.

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In-Depth Study of Copper Selenide Synthesis using the Pack Cementation Technique

V. Pavlidis[1], A. Teknetzi[1], D. Stathokostopoulos[1], E. Tarani[1], C. Papoulia[1], S. Hadjipanteli[2], Th. Kyratsi[2], G. Vourlias[1]

[1]School of Physics, Faculty of Sciences, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece
[2]Dept. of Mechanical and Manufacturing Engineering, University of Cyprus, Nicosia 1678, Cyprus

Thermoelectric technology, which directly converts waste heat into electricity, could play a crucial role in addressing the energy and environmental crisis. Traditional thermoelectric materials face limitations due to cost, toxicity or the scarcity of their constituent elements. Recently, β-Cu_2Se has attracted significant attention. This is due to its promising thermoelectric properties and unique ion-liquid behavior of Cu ions within the selenium lattice framework, resulting in a high figure of merit (up to at least ZT=1.6) in the temperature range of 500-800 °C.

In this research, the synthesis of copper selenide using the Pack Cementation technique is studied. Specifically, by varying the synthesis time and stoichiometry or introducing an additional heating step, the optimal synthesis conditions for thermoelectric Cu_2Se are investigated. The synthesis time was from 1 hour to 4 hours at constant temperature (240 ºC), while the Cu:Se ratio varied from 2.0:1.0 to 1.8:1.0. The additional heating step was at 350 °C for 30 minutes. The structure and crystalline phases of the samples were identified using XRD. The morphology and elemental composition were studied by SEM coupled with energy dispersive spectroscopy. The chemical state of the elements in the powders was investigated via XPS. The oxidation behavior of selected samples was examined by thermal tests using a thermogravimetric setup. Finally, the thermoelectric performance of the optimum material was evaluated through measurements of Seebeck coefficient, electrical conductivity and thermal conductivity.

A Cu:Se ratio of 2:1 resulted in incomplete synthesis with the presence of secondary phases (CuSe, Cu_3Se_2, Cu, Se) for all the tested synthesis times. By reducing the copper content and introducing the additional heating step, the thermoelectrically preferred β-Cu_2Se is enhanced. The synthesized Cu_2Se powder exhibited sufficiently good thermoelectric performance.

Designing Nanostructured Single-ion Polymer Electrolytes for Solid State Lithium Metal Batteries

Georgia Nikolakakou,[1,2] Christos Pantazidis,[3] Georgios Sakellariou,[3] Vasilis M., Papadakis,[1] Georgios Kenanakis,[1] Benoit Loppinet,[1] Emmanouil Glynos,[1,4]

[1]Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, P.O. Box 1385, 711 10 Heraklion, Crete, Greece
[2]Department of Chemistry, University of Crete, P.O. Box 2208, 710 03 Heraklion, Crete, Greece
[3]Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografrou, 15 771 Athens, Greece
[4]Department of Materials Science and Engineering, University of Crete, P.O. Box 2208, 710 03, Heraklion, Crete, Greece
Email: eglynos@iesl.forth.gr

Abstract:

Single-ion s~~S~~olid polymer electrolytes (SI-SPEs) hold the key for the realization of high energy-density Li-metal batteries, as they are chemical stable towards Li metal while their mechanical resistance could reduce, or even suppress Li dendrite formation and eliminate the associated safety hazards and the catastrophic failure of the battery.
Despite the considerable research effort in SI-SPEs, the development and realization of their potential has been hampered by the inability to design materials that possess simultaneously, high ionic conductivity, good mechanical properties, and a cation transference number close to unity

We will outline our recent research effort towards the design of high-performance SI-SPEs. In particular, we will introduce the use of novel, stiff/glassy, polyanion nanostructured polymer particles, as (i) single-component nanostructured materials, where the entire SI-SPEs will be created by the polyanionic particles ~~nanoparticle~~ as building blocks and (ii) as additives to liquid, low molecular weight, liquid, fast conducting polymer electrolytes. Key of this approach is the fact that the morphology of the resulting SI-SPEs may be precisely controlled through changes in the molecular architecture and composition of the nanostructured polymer nanoparticles, directing either their dispersion or their self-assembly into highly interconnected structures. This novel approach for the synthesis of nanostructured materials, with tailored/on-demand structures and electrochemical properties offers new ways to control the morphology of SI-SPEs and to decouple and tune the antagonistic properties of ion-conductivity and shear modulus, which currently limits the realization of single-ion polymer electrolytes in lithium metal batteries.

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Synthesis of fluorescent copper nanoparticles in the presence of amine containing polymers

S. Amarantos[1,2], D. Vagenas[1], G. Mousdis[1], S. Pispas[1]*
[1] Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., 11635 Athens, Greece
[2] Department of Materials Science Engineering, University of Ioannina, University Campus-Dourouti, 45110 Ioannina, Greece.

Abstract: In this work copper nanoparticles were synthesized using amine containing polymers as reducing agents and stabilizers. The polyelectrolytes utilized were hyperbranched polyethyleneimine (H-PEI), linear poly [2-(dimethylamino) ethyl methacrylate] (PDMAEMA) and chitosan (Chi). The synthesis takes place in a one-step reaction in the absence of a highly reactive reducing agent, at relatively low to medium temperatures and in aqueous solution. In addition to the effect of temperature, in the range 60-140ºC during nanoparticle synthesis, on the physicochemical and structural properties of the nanocomposite Cu-polymer particles was examined. The obtained nanoparticles were characterized through UV–vis (UV-vis) and fluorescence (FS) spectroscopy, dynamic and electrophoretic light scattering (DLS, ELS) and transmission electron microscopy (TEM). The Cu-nanocomposites were irradiated at wavelengths from 300nm to 500nm and exhibited interesting fluorescence properties. In parallel they were studied regarding their size depending on the polymer stabilizer and the temperature of synthesis. Their temporal stability was also examined during the course of two weeks and from the data collected the nanocomposites may be considered as good candidates for applications concerning bioimaging and antibacterial activity.

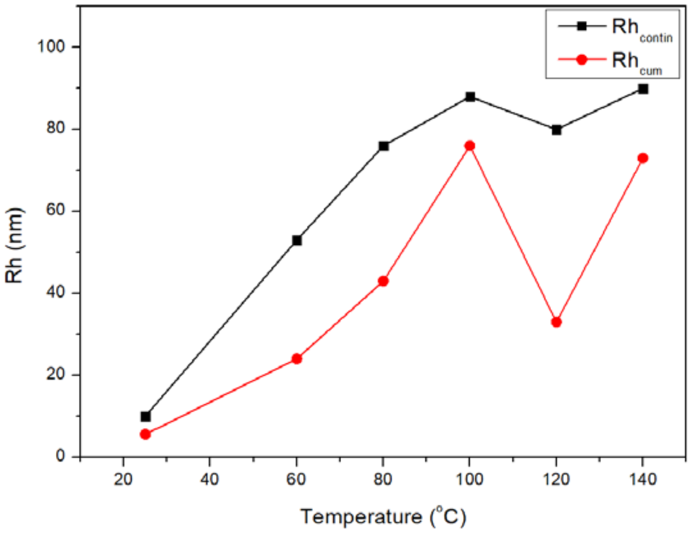

Figure 1 : schematic representation of the change in hydrodynamic radius of the nanocomposite as a function of the synthesis temperature

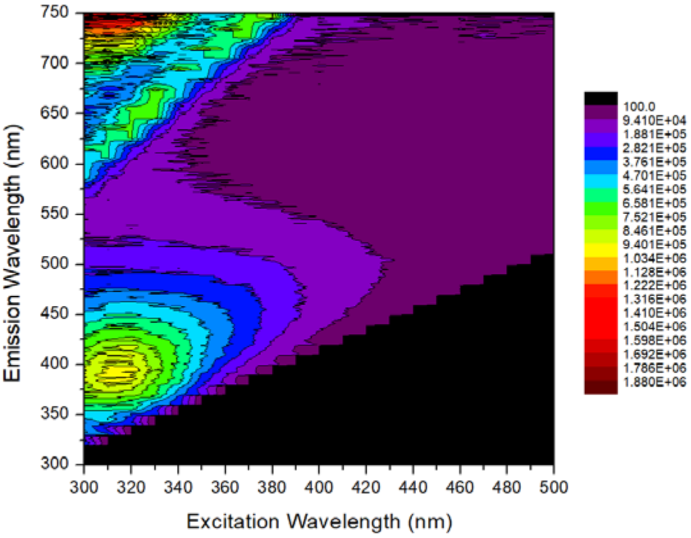

Figure 2 : Three dimensional fluorescent diagram of Nanocomposite

Design of metallic materials for biocompatible applications

Nousia M. E., Pavan C., Scaglione F., Turci F., Rizzi P.

University of Turin, department of Chemistry, NIS and INSTM, Via Pietro Giuria 7, 10125 Torino, Italy

With the increasing life expectancy the need for biomaterials, and implants in particular, has risen. Even though the commercial Ti alloys used today as hard tissue replacements showcase good short-term properties, they tend to fail long term because of not sufficient corrosion resistance, release of cytotoxic elements, difference between the elastic moduli of the implant and the human bone, and poor resistance in biofilm formation on their surfaces. [1] To tackle this problem, designing new β-Ti alloys and engineering their surfaces is of great importance, as it allows to achieve the desired interaction with the body eliminating poor osteointegration, reduction of bone mass, biofilm formation and implant related infections. [2]

In this work, two low Young modulus β-Ti alloys were studied, Ti-24Nb-4Zr-8Sn (%wt) and Ti-45Nb (%wt), that do not contain toxic elements. The alloys were prepared by arc-melting in argon atmosphere. To ensure homogenization, the alloys underwent a heat treatment, at 1000° for 24h.

The surfaces of the β-Ti alloys were hydrothermally treated to create micro- and nano-patterned surfaces. SEM and XRD analysis were carried out to assess the alloys' microstructure and surface morphology, while contact angle measurements were followed to evaluate their hydrophilicity. Different types of surface patterns were observed for the different types of solutions that were used during the treatments. When an acidic solution was used, titanium oxide micro-spheres formed a microporous surface layer, with a contact angle of 80°, whereas when a basic solution was used, the oxide layer has nano-grass like structure and a contact angle of 15° making it super-hydrophilic.

Following the modification treatments, studies on the hemo- and bio-compatibility of the materials were carried out using hemolysis assay (HA) and simulated body fluids (SBF).

These features are a promising way to achieve the desired implant surface-cell interaction, as osteoblast adhesion onto the surface.

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Metal content and Fe bonding in mussel byssus from different aquatic environments

E. Proiou[1], A. Staikou[2], E. Paloura[1], K. Simeonidis[1], M. Katsikini[1]
[1]Aristotle University of Thessaloniki, School of Physics, Physics, 54124 Thessaloniki, Greece
[2] Aristotle University of Thessaloniki, School of Biology, 54124 Thessaloniki, Greece

Abstract: Bivalves create bundles of filaments, called byssus, whose primary purpose is to enable their stable attachment to rocks or other surfaces. The mechanical properties of byssus have attracted scientific interest, mainly due to their formation mechanism, structure, and function as well as in biomimetics. Byssal threads are rich in metals, such as Fe, Mn, Cu, and Zn, with their concentration being affected by the growth environment. The metals have a key role in self–healing and give to the byssal threads remarkable mechanical properties via their complexation with amino acids or DOPA (3,4-dihydroxyphenyl-L-analine). This study focuses on the metal content and the bonding environment of Fe in byssuses obtained from mussels collected from 7 different aquatic environments. Some individuals lived shortly in aquaria filled with seawater, pure or rich in Fe, Zn, Cu or Mn (metal chlorides were used to prepare the solution) before the collection. In addition, some byssus bundles, after being detached from the mussels, were stored in solutions with a high concentration in metal ions. X-Ray Fluorescence (XRF) and X-Ray Absorption Fine Structure (XAFS) measurements were conducted at the XAFS beamline of ELETTRA. A representative XRF spectrum recorded from a byssus sample is shown in Fig. 1. The presence of various metals is evident. To quantify the metal concentration, the mass ratios of Ca, Ni, Cu, Zn and Mn to Fe were determined. The bonding environment of Fe was accessed using XAFS spectroscopy. Representative Fourier Transform (FT) of the Fe-K-edge EXAFS spectrum, along with the XANES spectrum in the inset, is shown in Fig.1. The pre-edge peak in the XANES spectra reveals that Fe is trivalent and octahedrally coordinated. However, slight variations in the position of the absorption edge and the shape of the spectrum at energies beyond the absorption edge reveal modifications in the Fe bonding environment which are also evident in the FT of the EXAFS spectra.

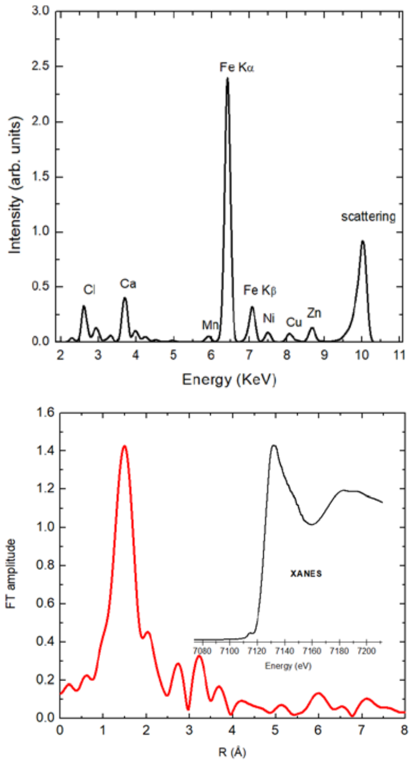

Fig.: (top) Representative XRF spectrum of a byssus; (bottom) Fourier transform of the Fe-K-edges EXAFS spectrum and XANES spectrum in the inset.

The role of vacancies in β-TiCuZr dealloying by ab initio calculations

Nousia M. E.[1,2], Tiwari K.[2], Rizzi P.[1], Lekka Ch. E.[2]

[1]*University of Turin, department of Chemistry, NIS and INSTM, Via Pietro Giuria 7, 10125 Torino, Italy.*
[2]*Department of Materials Science & Engineering, University of Ioannina, Ioannina, Greece*

Dealloying mechanism in metallurgy corresponds to a selective dissolution of less noble elements from an alloy that usually results in a nanoporous material [1]. Treating the surface of a biocompatible alloy like β-TiZrCu by dealloying might result in desirable antibacterial non-toxic features by reducing or tuning the Cu concentration. Aiming to understand the early stage of dealloying, selective atoms were removed from the β-$Ti_{40}Cu_{40}Zr_{20}$(at%) surface and the vacancy formation energy was calculated starting from the pure Cu (fcc), Ti (hcp) and Zr (hcp) low index (001) surfaces. It cases out that the Cu surface vacancy formation energy (0.857eV) is lower than the bulk one (1.24eV) in line with previous calculations (1.09eV) [2] which suggests that a Cu atom requires less energy to be removed from the surface layer. In addition, the Cu vacancies are favoured against Ti and Zr vacancies [2], [3].

In the β- $Ti_{40}Cu_{40}Zr_{20}$(at%) several surface structures and configurations have been investigated resulting the rich in Cu terminated layer as the energetical favoured. In accordance with the experimental results of an amorphous $Ti_{40}Cu_{40}Zr_{20}$ structure, the surface structure that has been found to be energetically favoured is the agglomerated Ti and Cu configuration having mixed Zr atom’s first neighbourhood. The metallic character of the alloy is maintained throughout the surface while non-bonded 3d orbitals are observed, especially on Cu atoms, creating dangly bonds.The vacancy formation energy in the Cu neighbourhood is lower than the ones of Ti and Zr, which suggests that a Cu atom requires less energy to be removed from the surface layer.

The results of the present work could be used for the understanding of the dealloying mechanism’s first stages and the formation of a nanoporous surface of a Ti-Cu implant for orthopaedic and dental applications.

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Synthesis and Characterization of Novel Linear Triblock Copolymers

S. Tsirkas[1], G.-M. Manesi[2], A. Avgeropoulos[3]
[1]*Department of Materials Science Engineering, University of Ioannina,*
University Campus-Dourouti,45110 Ioannina, Greece

Triblock copolymers with rigid polystyrene (PS) core and poly(dimethylsiloxane) containing (PDMS) side arms of the PDMS-*b*-PS-*b*-PDMS sequence were synthesized using living anionic polymerization techniques under high vacuum conditions. A platform methodology combining well-established synthetic protocols is proposed for the synthesis of the specific triblock copolymers for the first time in literature allowing the preparation of well-defined materials with narrow distributions and controlled molecular characteristics.

The objective of the specific research was to study the structure/properties relationship when the amorphous rigid block constitutes the core and the soft crystalline segment the outer chains. The ability to tune the sequence of segments is expected to induce various structures which will be affected not only by the composition, repulsive energy and total degree of polymerization but also from the ability of the flexible chains to curve due to covalent junction on the rigid PS core. In addition, the PS/PDMS systems showcase intriguing properties and potential for various applications including nanotechnology and electronics.

The synthesis of the PS core was based on sodium-napthalenide reagent which was utilized as the difunctional initiator and provides a very fast initiation step due to the electron transfer that occurs from sodium to naphthalene. To conjugate the middle difunctional block with the living PDMSLi$^+$ macroanions which were independently synthesized, an appropriate linking agent, namely dimethyldichlorosilane was selected.

The molecular characterization of the polymers was performed with size exclusion chromatography (SEC), mebrane osmometry (MO) and proton nuclear magnetic resonance spectroscopy (^{1}H-NMR). The thermal analysis of the polymers was accomplished using differential scanning calorimetry (DSC) and the morphological characterization with transmission electron microscopy (TEM). A systematic comparison between the structures obtained from the PDMS-*b*-PS-*b*-PDMS and PS-*b*-PDMS-*b*-PS copolymers with similar molecular characteristics was carried out in order to justify how the alternation of block sequence may affect the structure/properties relationship.

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Exploiting "Soft Matter": Well-Oriented Cubic Lattice Network Morphologies Tuned from Triblock Terpolymers Systems

K.Artopoiadis[1], G.-M. Manesi [1], I.Moutsios[1], A. Avgeropoulos [1]
[1]Department of Materials Science & Engineering, University of Ioannina, Dourouti University Campus 45100 Ioannina, Greece

Block copolymers undeniably, have created a major impact in the scientific research community rendering them as ideal candidates for numerous nanotechnological applications. The inherent ability of these materials, to self-assemble in bulk state or in selective solvent environment has led to well-ordered nanostructures with well-defined periodicities.

The unique ability of enabling controlled polymerization techniques to precisely engineer and design well-defined block copolymer and terpolymer systems is of paramount importance. By regulating the sequence of each segment and manipulating the molecular, compositional and architectural characteristics, we are able to intervene and alternate the final adopted morphology in bulk. In accordance with the previous, a triblock terpolymer system comprised from three chemically incompatible segments (ABC or BAC) since the sequence of the AB blocks can be altered, resulting in the complete differentiation of the inherent properties the two systems exhibit and can be investigated. The main goal in this system is to efficiently add up an amorphous (PS), an elastomeric segment (PB of either 1,2 or 1,4 microstructure) with a silicon containing segment (PDMS) and study the morphological behaviour and the self-assembly of this system showcased in bulk state.

The final materials were molecularly characterized via size exclusion chromatography (SEC) and Proton nuclear magnetic resonance spectroscopy (^{1}H-NMR) indicating molecular and compositional homogeneity correlated with narrow polydispersity indices as expected. Additional thermal characterization was conducted via differential scanning calorimetry (DSC) assisting in a two-fold manner: a)the assessement of, at least, the glass transition temperatures (Tg) corresponding to each segment and b) a prominent evidence of an efficient microphase separation prior morphological studies. In order to probe the structure/properties relationship transmission electron microscopy (TEM) and small angle X-ray Scattering (SAXS) were employed unveiling cubic periodic network morphologies with sub-10nm total periodicities necessitating the use of these materials in nanotechnology and nanopatterning applications.

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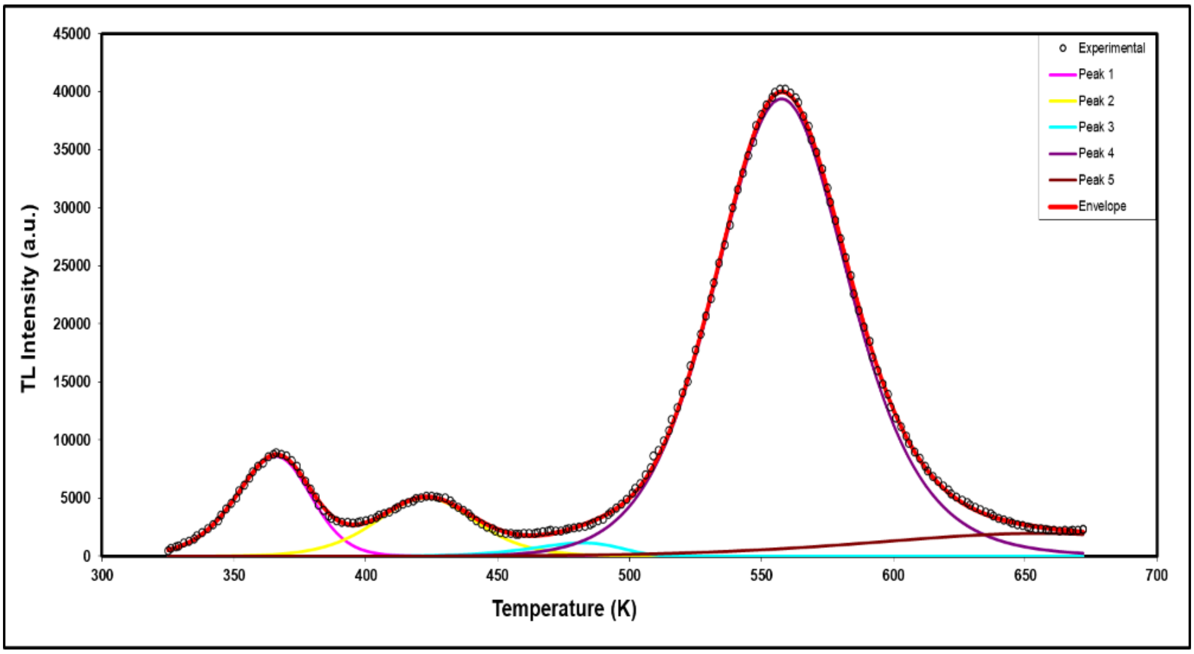
Investigating the Thermoluminescence Properties of commercially available ultramarine pigments

A. Pourliaka[1], I.K. Sfampa[2], L. Malletzidou[3], G. Kitis[2], G. Vourlias[1]
[1]*Laboratory of Advanced Materials and Devices, School of Physics, Faculty of Sciences, Aristotle University of Thessaloniki, Thessaloniki, GR- 54124, Greece*
[2]*Nuclear and Elementary Physics Laboratory, School of Physics, Faculty of Sciences, Aristotle University of Thessaloniki, Thessaloniki, GR- 54124, Greece*
[3]*Laboratory of Archaeometry and Physicochemical Measurements, Athena Research Center, Kimmeria University Campus, GR-67100, Xanthi, Greece*

Abstract: Ultramarine is considered as a valuable pigment, because of its exceptional color, longevity, and inherent worth. The rare semiprecious stone lapis lazuli, was used traditionally to produce the blue pigment Ultramarine. Lapis lazuli is a complex of minerals, the main mineral phase in the rock is lazurite, which is a mineral sulphide of calcium and sodium, with chemical formula $(Na,Ca)_8(AlSiO_4)_6(SO_4,S,Cl)_2$ and belongs to the category of sodalite minerals, part of the broad category of feldspathoid group[1,2]. Authenticity verification and precise, direct dating of artworks are crucial challenges in archaeometry. Thermoluminescence (TL) stands among the basic research tools in the fields of ionizing radiation dosimetry, archaeological dating and generally, retrospective dosimetry. The TL properties of two different commercially available ultramarine pigments whose raw material comes from two different regions of South America have been thoroughly studied, to evaluate their potential use as TL dosimeters, which could aid in authentication studies or dating artifacts. TL measurements were carried out using a Harshaw 3500 TLD-Reader. The irradiations were applied through a ^{90}Sr/^{90}Y beta particle source. All measurements were performed in a nitrogen atmosphere with a low constant heating rate of 2ºC/s and the samples were heated up to the maximum temperature of 400 °C. The main properties studied included the glow-curve shape, the sensitivity to ionizing radiation and the sensitization after repeated irradiation-measurement cycles, along with the estimation of the lower detectable limit. Moreover, the Single Aliquot Regeneration (SAR) protocol was employed, which is suitable for high value samples due to its minimal quantity requirement[3,4]. Finally, the potential fading of the luminescence signal as a function of time between irradiation and measurement was investigated.



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Microwave assisted method for cellulose nanocrystals isolation from Aloe vera plant residue for potential use for biomedical applications

Eleni Triantafyllou[1], Christina Kyriakaki[1], Andreas Karydis-Messinis[1], Dimitrios Moschovas[1], Constantinos E Salmas[1], Apostolos Avgeropoulos[1], Nikolaos E Zafeiropoulos[1]

[1]Department of Material Science Engineering, University Campus-Dourouti, Ioannina, 45110, Greece

Abstract: Cellulose nanocrystals are a promising material due to their mechanical properties as well as their ability to biodegrade. In this study, a new approach regarding the isolation of cellulose nanocrystals from Aloe plant residues is presented and for this purpose the Microwave assisted method will be used. Aloe is a great source of cellulose which enables the creation of materials with a low environmental footprint. This extraction method accelerates the conversion of biomass into cellulose, improving the performance of the final material, reducing processing time as well as energy consumption, making it a viable option to produce biofuels, packaging materials and materials for biomedical applications. Characterization of the extracted cellulose and cellulose nanocrystals was carried out using various techniques, including scanning electron microscopy (SEM), X-ray diffraction (XRD), and Fourier-transform infrared spectroscopy (FTIR). The results confirmed the successful isolation of CNCs with a high aspect ratio and crystallinity.

As already investigated, the potential applications of extracted CNCs are many covering several fields. It has been shown that nanocrystals have high material reinforcement properties when incorporated into biodegradable polymeric matrices and thus it follows that their potential use in biocomposite materials for various industrial applications.The development and utilization of CNC-based materials can contribute significantly to advancing sustainable technologies and improving human health.

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New spectroscopic methods for non-invasive pH sensing of aerosols

G.Theodoropoulos[1a], A.Psarelis[1a], A.Soto Beobide[1a], G.Mathioudakis[1a], Z.Lada[1a], C.Molina[1b], K.Andrikopoulos[1a,2], A.Nenes[1b,3] , G.Voyiatzis[1a]

[1]FORTH/ICE-HT, (a) LAMS & (b) CSTACC labs, GR-26504, Patras, Greece
[2]Department of Physics, University of Patras, GR-26504, Patras, Greece
[3]EPFL, Lab Atmospher Proc & their Impacts, CH-1015 Lausanne, Switzerland

Abstract: Airborne particles, or aerosols, originate from both natural and anthropogenic sources, with sizes ranging from a few nanometers to a few micrometers. Aerosols significantly impact human health, contributing to approximately 4.2 million premature deaths annually according to the World Health Organization (WHO). They also influence the climate through direct and indirect radiative forcing and affect terrestrial and marine ecosystems by supplying nutrients. The acidity (pH) of aerosols modulates nearly all of their properties and processes[1]. Despite its importance, aerosol pH has remained virtually unconstrained for decades. Recent developments have led to methods for inferring pH from measurements of gas and aerosol composition. These methods are now used globally but still face significant limitations. As a result, there is a strong need for accurate and direct determination of ambient aerosol pH.

The objective of this study is to propose a non-invasive strategy for monitoring the pH of aerosols. The methodology is based on the deposition of aerosol nanoparticles and microparticles on functionalized pH-sensitive filter surfaces, whose response is monitored via Raman/SERS measurements. The initial method employs a redox-active pH-responsive polymeric substrate, as a sensing material for the quantification of the acidity levels of aerosols (as well as of other environmental contaminants) that deposit on the substrate during normal sampling operations. The polymeric model system under investigation is polybenzimidazole (PBI), which undergoes protonation/deprotonation upon exposure to acids/bases, resulting in structural variations that exhibit distinct Raman fingerprints[2]. In addition, a second method is proposed. It includes low molecular weight pH-responsive molecules as surface modifiers of plasmonic nanostructures. It was found that the structural alterations caused by pH could be traced even at low concentrations through SERS measurements.

Keywords: Aerosols sensing, Raman Spectroscopy, pH responsive, atmospheric pollution

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Surface Characterization of Atomic Layer Deposited Inorganic Coatings on Polymeric/Biopolymeric Substrates.

A. Mouchtouris[1], E. Amirali[2], A. A. Barmpaki[1], L. Sygellou[2], P.K. Karahaliou[1], P. Svarnas[3] and C. A. Krontiras[1]
[1] *Department of Physics, University of Patras, Patras, Greece*
[2] *Institute of Chemical Engineering Sciences (ICE-HT), Foundation of Research and Technology, Patras, Greece*
[3] *Department of Electrical and Computer Engineering, High Voltage Laboratory, University of Patras, Patras, Greece*

Petroleum-based polymers, such as polyethylene (PE), polystyrene (PS) polypropylene (PP), polyethylene terephthalate (PET) etc., have undoubtedly prevailed in a wide range of applications, including food packaging [1]. However, their replacement by natural and synthetic analogues with significant bio-properties is one of the proposed actions that must be taken in order to eliminate the severe environmental impact of their use. Focusing on food packaging applications, systems based on polylactic acid (PLA) and polyhydroxybutyrate (PHB) have gained large attention in recent years [2-3]. In parallel, the surface modification of various biopolymeric substrates by inorganic coatings is of utmost interest. Towards this scope, our investigation deals with the inorganic coatings using the Atomic Layer Deposition (ALD) method, which provides uniform coatings with well-defined interfaces over the entire substrate area, at temperatures suitable for polymer substrates. Here, a few nanometers of Al_2O_3/ZnO bilayers were deposited on PLA, PHB and their blend, plasticized with epoxidized soybean oil methyl ester (ESOME), while ITO and PP were used as reference samples. The analysis was performed by X-ray Photoelectron Spectroscopy (XPS), a surface-sensitive technique that provides insight into the surface chemical modifications (C, O, Zn, Al), including atomic ratios and layer's thickness determination. In addition, chemical changes at the Al_2O_3/ZnO/polymer interfaces were elucidated. ZnO was used as an effective antimicrobial agent [4], while Al_2O_3 was used as a passivation layer, since, according to our previous work, the direct deposition of ZnO on PLA, results in the sub-surface diffusion of the used precursors and their reaction with PLA, creating a carbon-rich $Zn(OH)_2$ chemical state [5]. Water contact angle measurements were also performed to investigate the hydrophilic properties of the coated films.

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Optical and Dielectric Anisotropy of Laterally Fluorinated Liquid Crystalline Oligomers with two Nematic Phases

E.E. Zavvou[1], C. Welch[2], G.H. Mehl[2], A.G. Vanakaras[3] and P.K. Karahaliou[1]
[1] Department of Physics, University of Patras, 26504 Patras, Greece
[2] Department of Chemistry, University of Hull, Hull HU6 7RX, UK
[3] Department of Materials Science, University of Patras, 26504 Patras, Greece

Liquid crystal dimers consist of two mesogenic units linked via a flexible spacer. The elucidation of the structure–properties relationship in dimeric systems is highly topical due to the recent identification of spontaneous mirror symmetry breaking in a nematic fluid comprising achiral bent-shaped dimers with odd number of atoms in the spacer [1,2]. The novel, structurally chiral nematic phase, usually termed as N_{TB} or N_{PT} and herein as N_X phase, appears on cooling from the conventional nematic and is characterised by a nanoscale helical modulation of the local molecular orientational order [2,3]. While an overall bent molecular shape is considered a prerequisite for the manifestation of the N_X phase, the effect of the dipolar structure/correlations of the mesogenic units on the stabilisation of the mesophase is less understood.

This work comprises a comparative study of the optical and dielectric anisotropy of a laterally fluorinated liquid crystal dimer and its homologous trimer, both exhibiting two nematic phases. The effect of the number of linked mesogenic units on the magnitude of the optical and dielectric anisotropy in the high-temperature nematic phase is explored through comparative studies on the parent monomeric nematogen. In all studied systems the dielectric anisotropy has been determined in magnetically aligned samples, while birefringence measurements give valuable insights into the degree of ordering of the mesogenic units throughout the nematic phases. Comparison of the optical and dielectric anisotropies of the oligomers with the corresponding anisotropy of the monomer indicates a systematic variation of their magnitude with the number of the linked mesogenic units [4]. Results are also compared with the corresponding anisotropies of the cyanobiphenyl dimers [5–7], the archetypal compounds forming two nematic phases, and are discussed in terms of the dipolar structure of the mesogens and the dipolar correlations in their nematic phases.

Acknowledgments

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Cyanobiphenyl-based Liquid Crystal Dimers: the Effect of the Linking unit and Spacer length on the Emergence of Spontaneous Structural Chirality

E.E. Zavvou[1], W. Jiang[2], Z. Ahmed,[2] C. Welch[2], G.H. Mehl[2],
C.A. Krontiras[1], A.G. Vanakaras[3] and P.K. Karahaliou[1]
[1] Department of Physics, University of Patras, 26504 Patras, Greece
[2] Department of Chemistry, University of Hull, Hull HU6 7RX, UK
[3] Department of Materials Science, University of Patras, 26504 Patras, Greece

Liquid crystal dimers are composed of two mesogenic groups joined via a flexible spacer. The intrinsic flexibility of dimeric systems underlies their fascinating odd-even effects, i.e. the dependence of their transitional properties on the length and parity of the spacer [1]. Another manifestation of these well-known odd-even effects is the identification of spontaneous chiral symmetry breaking in a nematic fluid comprised of achiral dimers with exclusively odd number of atoms in the spacer [2,3]. The novel structurally chiral nematic phase, denoted herein as N_X, is typically obtained upon cooling from the conventional nematic and is characterised by a nanoscale periodic modulation of the local orientational order [3,4]. It is a common notion, that a prerequisite for the emergence of the N_x phase is the overall bent molecular shape. Considering symmetric dimers, this condition can be satisfied only for dimers with odd-numbered spacers, whereas the even-membered homologues are conventional nematogens [3,5].

In this work, we revisit the ether-linked CBOnOCB dimers with n= 5, 7, 9, 11 carbon atoms in the spacer, which, despite their overall bent shape and the obvious similarity with the archetypal N_X-forming CBnCB dimers, [6] are conventional nematogens. Nevertheless, their capability to participate in or sustain the formation of the N_X phase [7,8] has motivated us to conduct a systematic reinvestigation of their optical anisotropy, dielectric and conformational properties as a function of the spacer length. Results are compared with the methyl-linked dimer CB11CB, which exhibits two nematic phases, as well as with a corresponding monomeric nematogen. The optical anisotropy and dielectric response of the studied dimers are discussed in connection with their conformational properties, as well as with specific molecular features, providing valuable insights into their self-organisation in the nematic phase and into the specific conditions for the appearance of spontaneous structural chirality in nematic fluids.

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Open Innovation Modelling: MUSICODE Project

K. Kaklamanis, K. Kordos, M. Andrea, Ch. Trapalis, E. Lidorikis, D. Papagewrgiou
Department of Materials Science & Engineering, University of Ioannina
Ioannina 45110, Greece

Abstract: Modelling and simulation of organic optoelectronic materials and devices are important tools and accelerators of innovation. Validated models spanning multiple scales and domains of physics are coupled together creating a unique open innovation modelling ecosystem, i.e., an open innovation platform (OIP) for materials modelling. OIPs are intended to increase the EU industry competitiveness and its digital transformation. I'll present our recent activities in modelling optoelectronic devices, and our achievements in establishing an OIP through the H2020 MUSICODE project. The latter includes tools and methodologies for predicting/optimizing organic nanomaterials properties, relating structure-property to process conditions, designing/optimizing device functionalities, as well as a novel data management system facilitates its operation including a database of material and device property records, modelling workflow editing tools, interoperable modelling workflow execution, data analysis etc.

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http://musicode.eu/

Searching for Common and Individual Thermoluminescence Properties in Marble ($CaCO_3$) for Provenance Studies

A. Daglartzis[1], V. Melfos[2], G.S. Polymeris[3], G. Kitis[1]
[1]Physics Department, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
[2]School of Geology, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
[3]Physics Department, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

Abstract: The marble ($CaCO_3$), a common geological mineral, has been extensively utilized throughout human history. In ancient Greece, in particular, it was employed in constructing buildings and monuments, thus holding exceptional archaeological significance. Numerous physical methods contribute to uncovering crucial information about the provenance of ancient marble samples. In the case of Thermoluminescence (TL) the glow curve shape has been used as an identification method to characterize the individuality of ancient marbles. The present study goes further, having a twofold approach. Firstly, it investigates for global properties in one type of marble that can be extrapolated to all types of marble. Secondly, it examines properties individual to a specific type of marble that can serve as identifiers for that particular marble. The present work focuses on six marble samples originating from six Greek mines. The samples were categorized into two groups: (a) natural “as is” samples and (b) samples annealed at 800^0C for 1 hour and then rapidly cooled to room temperature. Measurements were conducted on (a) pieces of approximately 30 mg. (used as synthetic TL dosimeters) (b) powdered pieces, and (c) powder with dimensions of 80 – 140 μm. In all cases, ten successive irradiation readout cycles were conducted to evaluate the stability of the TL signal. For cases (a) and (b), measurements of the prompt isothermal decay at elevated temperatures were performed. Finally, for case (b) a complete TL dose response curve was obtained. These investigations provide insights into the defect states and trap depth distributions within the crystal lattice, which are critical for understanding the thermoluminescent properties of $CaCO_3$.

Optical profilometry for 3D mapping of optoelectronic devices

Savvas Sarigiannidis[1], Yannis Papadopoulos[1], Dimitrios G. Papazoglou[2, 3], Ioanna Zergioti[1]

1. Department of Physics, School of Applied Mathematical and Physical Sciences, National Technical University of Athens, 15780 Athens, Greece.
2. Institute of Electronic Structure and Laser, Foundation for Research and Technology Hellas, P.O. Box 1527, 71110, Heraklion, Greeee
3. Materials Science and Technology Department, University of Crete, P.O Box 2208, 71003, Heraklion, Greece

Abstract: The maximum number of words is 300, Type = 10 points, Font = Arial.

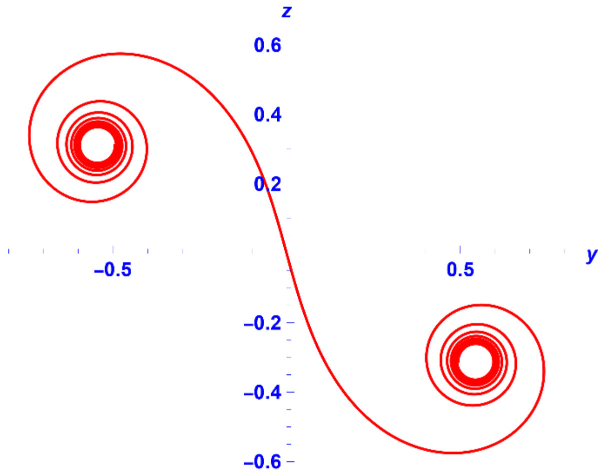
Photographs / graphics may be used if necessary to substantiate results.

Surface topography optical measurement techniques have emerged as an essential tool for microelectronics and photonics for online monitoring of the surfaces in the range of several microns up to a few mm. Specifically, lithographically produced patterns form step differences ranging from 10 to 300 nm relative to the underlying layers of the chip, which we need to know due to their importance regarding the performance of the chip. Amongst these techniques, phase shifting interferometry (PSI) is a non-contact topography technique, which uses the principle of light interference to deduce the difference in height of neighbouring areas. In this work, we present a compact approach which includes a Michelson-type optical profilometer aiming to measure patterned electrodes and waveguides on a silicon wafer. The setup consists of a laser source that provides both the illumination source and the coherent light source for fringe patterning, an imaging system with the appropriate magnification for the specific application at hand and the beam splitting element along with the reference mirror. For the most accurate results the Phase Shifting Interferometry (PSI) technique will be incorporated using a piezoelectric stage and software analysis. The developed setup can accurately measure step height differences of 100 nm, with a lateral resolution of ~30 μm and field of view of 2.0x0.8mm^2.

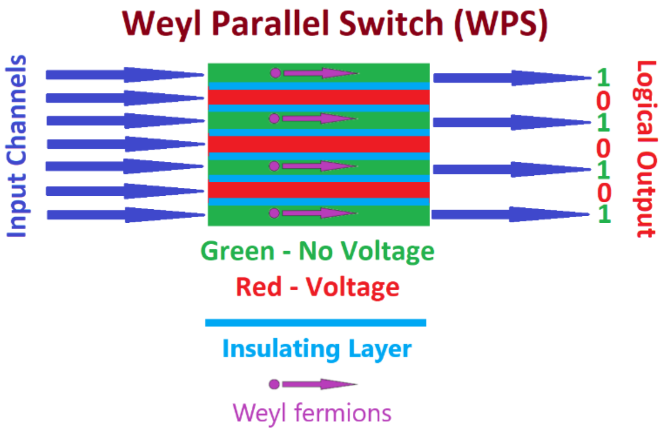
On the electromagnetic interactions of Dirac and Weyl particles

Georgios N. Tsigaridas[1], Aristides I. Kechriniotis[2], Christos A. Tsonos[2] and Konstantinos K. Delibasis[3]
[1]Department of Physics, School of Applied Mathematical and Physical Sciences, National Technical University of Athens, GR-15772 Zografou Athens, Greece
[2]Department of Physics, Postgraduate Program ‘’Applied Physics’’, University of Thessaly, GR-35100 Lamia, Greece
[3]Department of Computer Science and Biomedical Informatics, University of Thessaly, GR-35131 Lamia, Greece

Abstract: This work focuses on the electromagnetic interactions of Dirac and Weyl particles, showing that under special conditions they can exhibit extraordinary behaviour. Specifically, we have shown that all Weyl particles, and under certain conditions Dirac particles, can exist in the same quantum state under a wide variety of electromagnetic 4-potentials and fields, infinite in number, which are explicitly calculated [1]. We have also discussed a set of particularly interesting solutions to the Weyl equations, showing that Weyl particles can exist in localized states even in the absence of electromagnetic fields [2]. Furthermore, the localization of the Weyl particles can be easily adjusted using simple electric fields [2]. Based on these results we have proposed a novel device for controlling the flow of information at a rate of up to 100 Petabits per second using Weyl fermions [3]. These results are expected to find important applications in several fields of science and technology, such as nanophotonics, nanoelectronics, laser physics, solid state physics, etc., providing new pathways for further development in these fields, both in theory and applications.



Delocalization and relocalization of a Weyl particle using a simple electric field perpendicular to its direcyion of motion [2]



A proposed device for controlling the flow of information using Weyl particles [3]

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Hybrid Nonlinear Graphene–Gold Metasurfaces

A. Theodosi [1,2], O. Tsilipakos [3], A. Koulouklidis [2], I. A. Otoo [4], P. Kuzhir [4], S, Tzortzakis [1,2], M. Kafesaki [1,2]

[1] University of Crete, Department of Materials Science and Technology, Vasilika Vouton, GR-70013, Heraklion, Greece
[2] Foundation for Research and Technology Hellas, Institute of Electronic Structure and Laser, GR-70013, Heraklion, Greece
[3] National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, GR-11635, Athens, Greece
[4] University of Eastern Finland, Department of Physics and Mathematics, FI-80101, Joensuu, Finland
annatheodosi@iesl.forth.gr

Abstract: Graphene is an attractive two-dimensional material for nonlinear applications in the THz regime, due to its high third order nonlinearity and the ability to support tightly confined surface plasmons. In this work, we target a hybrid gold-patch/uniform-graphene metasurface implementation that is friendlier to an experimental demonstration compared to patterned graphene approaches and, at the same time, aims to further increase the efficiency of the third harmonic generation process. The efficiency of the nonlinear process is enhanced by spectrally aligning the fundamental and third harmonic frequencies with resonances of the metasurface, leading to spatiotemporal energy confinement in both steps, of excitation at ω and radiation at 3ω. Efficiencies as high as -15dB (3.2%) for input intensity 0.1 MW/cm2 are theoretically demonstrated. The nonlinear metasurface is fabricated and strong frequency shifts due to self-phase modulation are experimentally observed. These nonlinear shifts are verified by corresponding simulations. Our results highlight the potential of graphene-based metasurfaces for nonlinear applications.

Metasurfaces (MSs), ultrathin structures composed of a periodic arrangement of resonant meta-atoms on a plane, have attracted considerable research interest [1]. In order to enable nonlinear and reconfigurable, materials with intensity-dependent and tunable properties can be exploited in the meta-atom geometry. In this context, graphene is a unique nonlinear material for THz applications due to its strong third order nonlinearity in combination with the capability to support tightly-confined surface plasmons [2]. The short wavelength of propagating graphene plasmons enables the design of metasurfaces (MSs) supporting higher-order resonances, while the lattice constant remains subwavelength even for higher harmonic frequencies, avoiding diffraction effects. A proven approach for boosting the efficiency of third harmonic generation (THG) process is to carefully align the fundamental (FF) and third-harmonic (TH) frequencies with MS resonances, a strategy which has been termed double-resonant enhancement [3]. In our previous work [3], we studied MS structures where the graphene layer was patterned into rectangular patches and reported third harmonic generation conversion efficiency (CE) of -20dB (at input intensity of 0.1 MW/cm2) [4]. In this work, we target an implementation that is based on a uniform graphene layer and is, thus, friendlier to an experimental demonstration. The patterning, in the form of patches, is transfered to the underlying gold layer; this approach allows us to achieve strong resonances leading to enhanced conversion efficiency.

Our proposed MS [Fig. 1(a)] is composed of a uniform graphene layer on top of gold patches (with size αx × αy), rectangular in the optimal case, residing on a polymeric substrate (thickness h = 8.3 μm), backed by a gold backreflector. The lattice constant is a = 5.6 μm. To optimize the structure response, a parametric study with respect to the length and width of the patches, αx and αy, is performed. The CE [Fig. 1(b)] is calculated under continuous wave (CW) conditions with a frequency-domain finite element method by using two linear simulations, at the FF and TH frequencies, respectively [4]. The optimum point in the αx-αy map resulted in a conversion efficiency CE = -15dB (3.2%) for the Ex polarization. The power coefficients of the optimum metasurface with rx = αx/a = 0.90 and ry = αy/a = 0.65, obtained from plane-wave scattering simulations, are plotted in Fig. 2(a). The positions of the absorption maxima (black arrows) and the eigenfrequencies (red arrows) of the two resonances, are also marked on the spectrum. Furthermore, the maximum field enhancement factor (|Ex|/|Ex0|) at the plane of graphene is found to be ~10 for f = 4.0 THz and ~5 for f = 11.6 THz, as shown in Fig. 2(b). The field distribution of the Ex component as obtained from eigenmode analysis is plotted in Fig. 2(c).

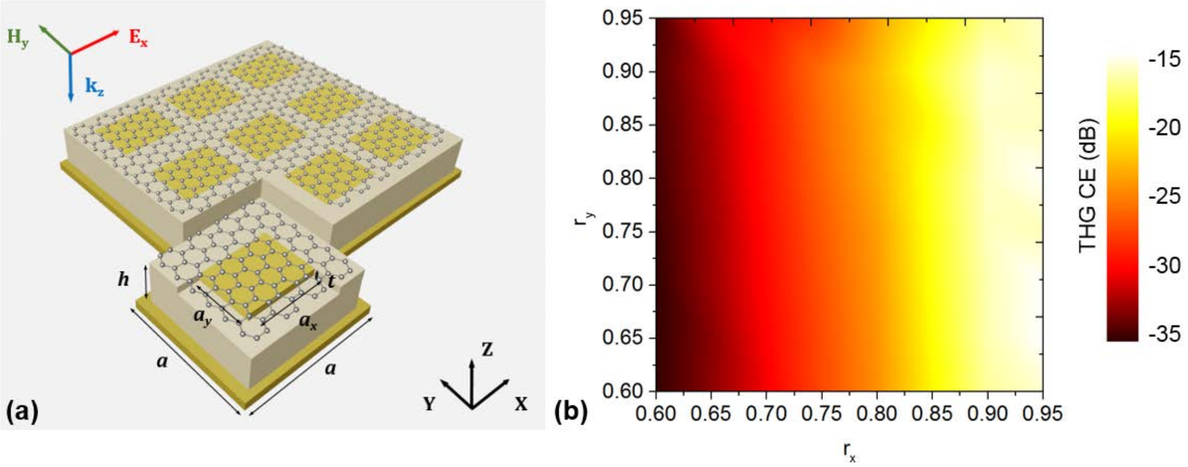

Fig. 1. *(a) Schematic of the hybrid gold-graphene metasurface. The metasurface is composed of gold patches ($a_x \times a_y$) with thickness t = 500 nm and electric conductivity σ = 4 × 10^7 S/m, placed in a square periodicity with period a = 5.6 μm, on top of a polymer substrate with relative electric permittivity $\varepsilon_r = 3.2 \times (1 - j0.1)$ and thickness h = 8.3 μm, backed by a gold backreflector. The incident wave is is linearly polarized along the x-axis. A uniform graphene layer is placed on top of the metasurface. (b) Calculated Third Harmonic Generation conversion efficiency under continuous plane wave illumination at normal incidence, for input intensity 0.1 MW/cm^2, as a function of the gold patch size: $a_x = r_x \times a$ and $a_y = r_y \times a$.*

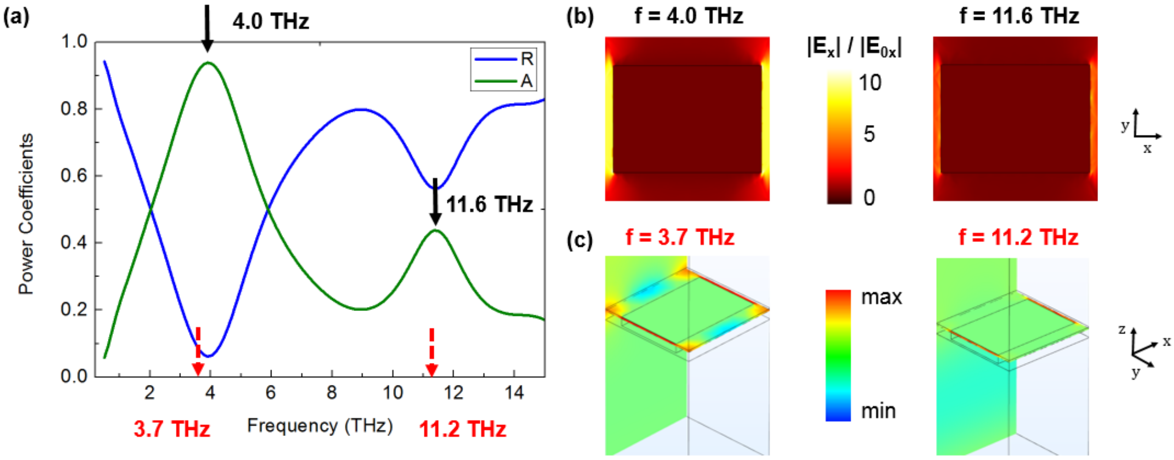

Fig. 2*. Analysis of the optimum metasurface with rx = 0.90 and ry = 0.65. (a) Reflection (R) and absorption (A) power coefficients of the double resonant metasurface obtained from linear plane-wave scattering simulations. The positions of the resonances are marked with black solid arrows and corresponding eigenfrequencies obtained from eigenmode analysis are marked with red dashed arrows. (b) Field enhancement factor |Ex| / |Ex0|, calculated at the plane of graphene. The maximum field enhancement factor is calculated to be ~10 for the first resonance and ~5 for the second. (c) Field distribution of Ex component obtained from eigenmode analysis.*

The graphene-gold metasurface discussed above was fabricated using e-beam lithography (the sample is shown in the inset of Fig. 3(a)) and an initial electromagnetic characterization has been performed. For the electromagnetic characterization we employed THz time domain spectroscopy. After transforming to the frequency domain, the reflection coefficient for different incident field strengths (temporally averaged across the entire duration of the pulse) is depicted in Fig. 3(a). We observe a strong nonlinear frequency shift of the structure resonances (especially of the lower-frequency one) due to self-phase modulation. The corresponding simulations are shown in Fig. 3(b) and are in good agreement with the experimental measurements. Additional measurements, involving modifying the experimental set-up so as to allow investigation of the THG in the structure are in progress.

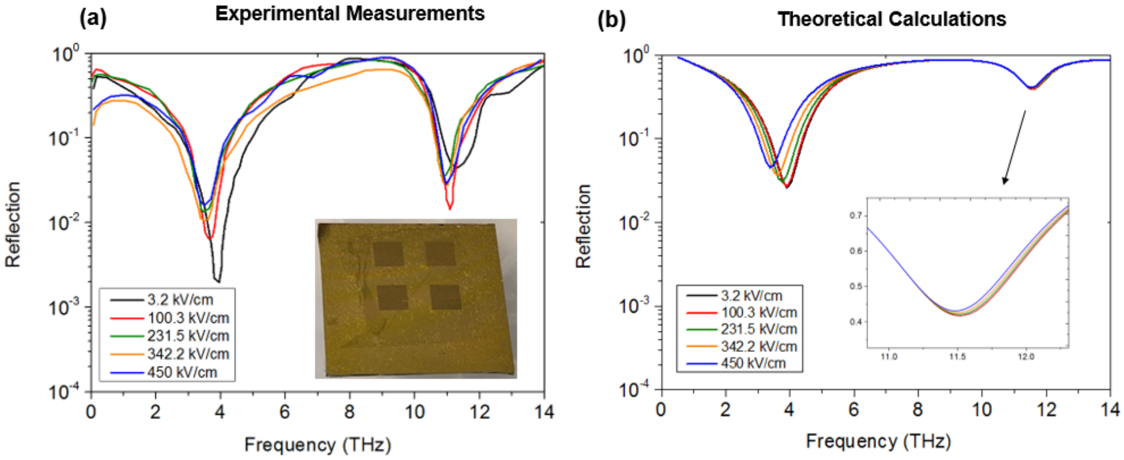

Fig. 3. *(a) Experimental reflection spectra of the fabricated non-linear hybrid gold-graphene metasurface (shown in the inset) as a function of the incident electric field strength; (b) corresponding to (a) theoretical calculations (the frequency shift of the second resonance is shown in the inset).*

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XANES spectroscopy study of temperature induced Fe spin state transitions in Fe-triazole nanoparticles

E. Petsali[1], F. Pinakidou[1], V. Tangoulis[2], N. Lalioti[2], F. D'Acapito[3],
E. C. Paloura[1], M. Katsikini[1]

[1] Aristotle University of Thessaloniki, School of Physics, 54124 Thessaloniki Greece
[2] University of Patras, Department of Chemistry, Laboratory of Inorganic Chemistry, 26504 Patras, Greece
[3] CNR-IOM-OGG, c/o ESRF LISA CRG, Avenue des Martyrs 71, 38000 Grenoble, France

Spin crossover compounds have emerged as versatile materials with applications spanning over various scientific and technological domains including magnetic sensors, data storage devices, and thermally responsive agents in Magnetic Resonance Imaging (MRI) [1]. In this study, we focused on Fe-triazole (Trz) nanoparticles where Fe^{2+} is octahedrally coordinated with Trz ligands forming polynuclear chain-like complexes. The silica coated Fe^{2+}-Trz nanoparticles exhibit the spin crossover effect which refers to alteration in the Fe spin state from low (LS) to high (HS) spin and can be triggered by an external stimulus such as temperature. This LS to HS transition is reversible but exhibits hysteresis. Here we apply temperature dependent Fe-K-edge X-ray Absorption Near Edge Structure (XANES) spectroscopy for the study of the alterations in the Fe unoccupied electronic states and local symmetry upon temperature induced Fe spin state transitions. The nanoparticles were synthesized by a reverse micelle technique and have diameters ranging from 10 to 50 nm [2]. The Fe-K-edge XAFS spectra were recorded at the LISA beamline of the ESRF in transmission mode in the temperature range 300 - 470 K. It is shown that the maximum intensity of the spectrum in the range 7125-7130 eV can be used as a means for the assessment of hysteresis.

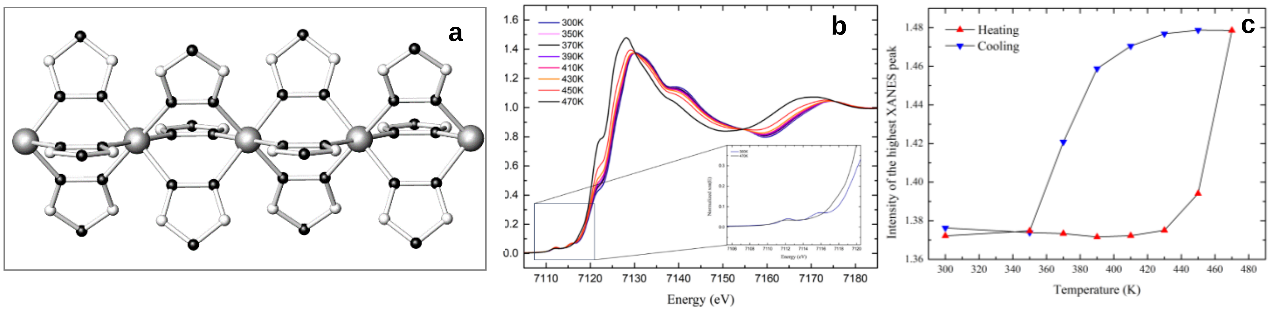

Fig.1 (a) Schematic representation of the Fe-Trz chains in the samples. (b) XANES spectra recorded upon sample heating from 300 K to 470K. The pre-edge region of the spectra recorded at 300 K and 470 K is shown in the inset. (c) Plot of the maximum intensity of the XANES spectra as a function of temperature. Red and blue symbols correspond to temperature increase and decrease, respectively.

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Graphene-based saturable absorbers in waveguide integrated schemes

A. Pythara[1], V. Nousia[2], S. Doukas[2,3], E. Lidorikis[2]
[1]*Department of Physics, University of Ioannina, Ioannina 45110, Greece*
[2]*Department of Materials Science & Engineering, University of Ioannina, Ioannina 45110, Greece*
[3]*Department of Physics, National and Kapodistrian University of Athens, Athens 15784, Greece*

Graphene has emerged as a promising material for saturable absorbers, with its unique non-linear optoelectronic properties enabling a wide range of applications in ultrafast photonics and laser technology [1]. Accurate simulation of the optical response of graphene under intense illumination is essential for designing devices for pulse-shaping, mode-locking and Q-switching towards the generation of ultra-short laser pulses. Here, we utilize our self-consistent multiphysics computational framework [2-5] that describes graphene's optical response upon intense photoexcitation in photonic integrated schemes. We explore the inclusion of graphene in CMOS-compatible Si-based waveguide cavities and racetrack resonators, while self-consistently accounting for its optical, electrical and thermal dynamic response under photo-excitation with *ps* pulses. By exploiting the interplay between critical coupling [2] and absorption saturation effects [1], we aim to design all-optical modulators and showcase the pulse-reshaping effects in waveguide-integrated configurations. We investigate and compare the performance of waveguide-cavity and racetrack-resonator graphene-based devices, in terms of response speed and saturation intensity, with the scope of designing graphene-based saturable absorbers in photonic-integrated schemes that can be utilized in waveguide-integrated laser systems.

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Electrical detection of van der Waals polaritonic nanoresonators at mid-infrared

Ioannis Vangelidis[1], Sebastián Castilla[2], Yuliy Bludov[3], Nuno Peres[3], M.I. Vasilevskiy[3], Frank H. L. Koppens[2], Elefterios Lidorikis[1]
1 University of Ioannina, 45110, Ioannina, Greece
2 ICFO, 08860, Castelldefels (Barcelona), Spain
3 University of Minho, Braga, Portugal

Abstract: Polaritons are hybrid excitations resulting from the coupling of light and free charge-carrier oscillations (plasmons) or lattice vibrations (phonons). In two-dimensional (2D) materials, polaritons are characterized by a number of fascinating properties like long lifetimes, extreme light confinement, and adjustable interactions. Despite their well-studied optical properties, the infrared photocurrent spectroscopy of polaritons has yet to be studied. In this work, we used a self-consistent multi-physics modeling framework, including optical, thermal, and electrostatic simulations, to study a novel experimental device that merges the polaritonic medium and photodetector into the same platform, as shown in Figure 1[1]. Metallic gratings were used to match the momentum of hybrid nanoresonators in a 2D polaritonic system (hBN/SLG/hBN stack) in the mid-infrared, and their response was electrically detected. The nanoresonators showed excellent quality factors (up to 200) [1]. Our simulations revealed various phenomena, such as the hybridization of graphene plasmons and hyperbolic phonon-polaritons (HPPs) in hBN, the tunability of the polaritons by graphene doping, and the interaction between distinct graphene plasmons (surface and acoustic). These findings were successfully verified through optical and photocurrent spectroscopy measurements. By accurately predicting the spectral photoresponse of this hybrid system and its excellent comparison to experimental data, we demonstrated that polaritonic materials can be used in novel sensing and photodetection platforms.

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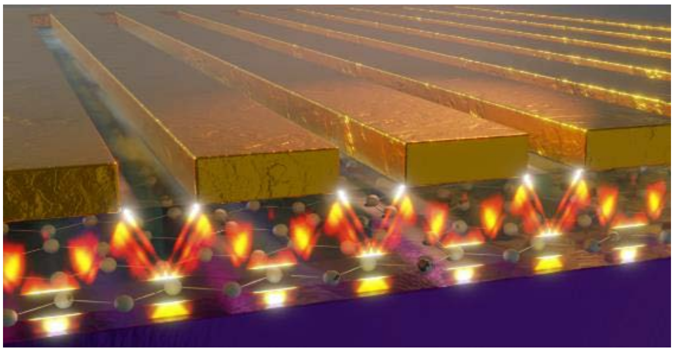

Figure 1: Schematic of the 2D polaritonic platform that shows the field intensity of the propagating HPP propagating mode.

Acknowledgement
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A self-consistent simulation framework for modelling graphene-based optoelectronics in the THz regime

S. Doukas[1,2], A. D. Koulouklidis[3], S. Tzortzakis[3], M. Kafesaki[3,4], E. Lidorikis[2], A. C. Tasolamprou[1,3]

[1] Department of Physics, National and Kapodistrian University of Athens, Athens 15784, Greece
[2]Department of Materials Science and Engineering, University of Ioannina, Ioannina 45110, Greece
[3]Institute of Electronic Structure and Laser, Foundation for Research and Technology Hellas, 71110, Heraklion, Crete, Greece
[4]Department of Materials Science and Technology, University of Crete, Heraklion, 70013, Greece

Graphene, with its unique properties and tunability, can be integrated into metamaterial and metasurface configurations to realize novel optoelectronic schemes [1]. Among the most promising of these are graphene-based perfect absorbers [2], which can be utilized in all-optical, ultrafast modulators [3]. Besides tuning graphene's response via electrostatic gating [4], its absorption can also be modulated through self-actions when interacting with intense THz pulses [2,5].

In this work, we present a self-consistent multiphysics simulation framework [5,6] to model graphene's non-linear response to intense THz illumination. Our model accurately replicates the experimentally measured non-linear response of graphene-based thin film absorbers, unveiling the origins of ultrafast all-optical modulation in the studied devices [5]. These simulations provide insights into graphene carrier dynamics and facilitate the extraction of analytical relationships describing the device's response.

Furthermore, our ability to seld-consistently simulate graphene's electrical, optical, and thermal properties enables the design of configurations operating in the THz regime. This includes thin film absorbers and graphene-based metasurfaces, which have potential applications in spatiotemporal modulation, amplitude and phase modulation, harmonic generation, beam steering, and more [7].

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Enhancement of plasmo-photonic index sensor sensitivity by slow-light effects

E. Lampadariou[1], E. Chatzianagnostou[2, 3], D.V. Bellas[1], D. Spasopoulos[2,3],
J.-C. Weeber[4], N. Pleros[2,3], E. Lidorikis[1]

[1]Department of Materials Science and Engineering, University of Ioannina, Ioannina 45110, Greece
[2]Department of Informatics, Aristotle University of Thessaloniki, Thessaloniki, 54124, Greece
[3]Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Thessaloniki, 57001 Greece
[4]Laboratoire Interdisciplinaire Carnot de Bourgogne (LICB), Université de Bourgogne, Dijon, 21078 France
e.labadariou@uoi.gr

We present a systematic theoretical study of integrated plasmo-photonic Mach-Zehnder interferometers (MZIs) sensors decorated by Bragg cavity configurations. The Bragg cavities incorporate slow-light effects into the surface plasmon polariton (SPP) propagation, which enhance the SPP/analyte interaction and boost the sensor performance up to an order of magnitude compared to the corresponding undecorated one. The sensitivity is markedly elevated at the plasmonic band gap edges and within the coupled cavity bands, primarily due to the slow light effect. To thoroughly investigate the physics of these systems, we develop a simplified analytical model based on the transfer matrix method (TMM) and validate the findings by explicit 2D finite-difference time-domain (FDTD) simulations. Exploration of all design parameters provides the theoretical performance limits. This study establishes a detailed framework for optimizing slow-light plasmo-photonic sensors, underscoring their potential for significant advancements in biological and chemical sensing applications.

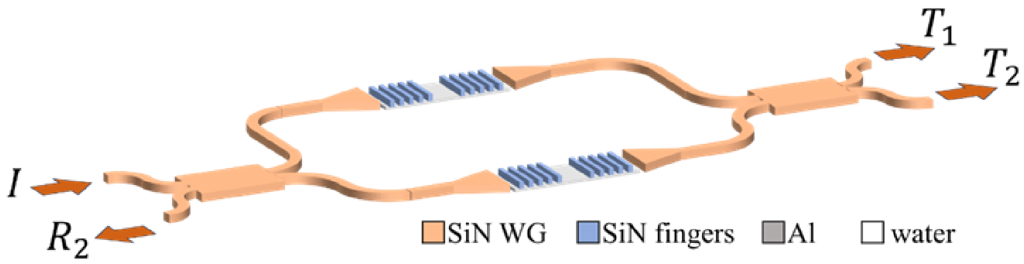

Fig. 1. Schematic of the proposed Bragg-assisted slow-light MZI plasmonic sensor.

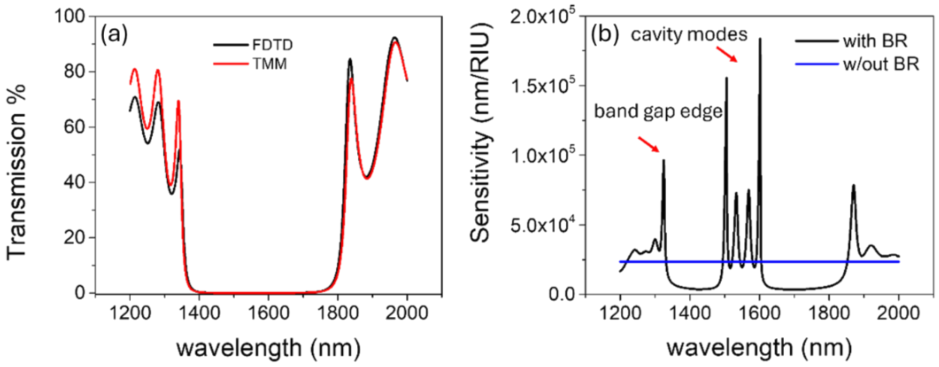

Fig. 2. (a) Comparison between the TMM and FDTD methods showing excellent agreement for the semi-infinite Bragg gratings. (b) Theoretical sensitivity of the Bragg plasmo-photonic sensor as a function of wavelength. The results for the corresponding undecorated bare plasmonic system are also shown for comparison.

Properties of mullite compacts obtained from diatomite

A. Šaponjić [1], S. Ilić[1], M. Pošarac-Marković[1], …
[1]*Department of materials, University of Belgrade, "Vinča" Institute of Nuclear Sciences National Institute of the Republic of Serbia, Mike Petrovića Alasa 12-14, Belgrade, Serbia*

Abstract:
Mullite compacts with excellent compressive strength have been fabricated using diatomite as Si and Al-nitrate as Al precursors with fibrous pore morphology. The hard mullite ceramics prepared by mold pressing without additives showed high compressive strength (up to 269 MPa, when sintered for 1h at 1500 ºC). Three temperatures (1300–1500 °C) were compromised between the obtained composition phases and the mechanical properties of analyzed compacts (1300, 1400, and 1500 ºC) for 1 h. The sintered samples at 1300 ºC showed that the crystalline mineral phases mainly comprise mullite, cristobalite, and corundum using XRPD. The presence of rod-like mullite grains with an aspect ratio 1:10 was confirmed by SEM analysis. XRPD of the sintered samples at 1500 ºC showed good mechanical stability and formation of pure mullite, making the analyzed diatomaceous earth suitable for producing various types of functional ceramic, and thermal insulating materials.

Influence of the Cation Chemistry on the Ion Transport Properties of PEO-based Polymer Electrolytes

Chrysostomos Papamichail, [1,2] Olympia Techlemtzi,[2,3] Georgia Nikolakakou,[2,3] Emmanouil Glynos,[1,2]

[1]Department of Materials Science and Engineering, University of Crete, P.O. Box 2208, 710 03, Heraklion, Crete, Greece
[2]Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, P.O. Box 1385, 711 10 Heraklion, Crete, Greece
[2]Department of Chemistry, University of Crete, P.O. Box 2208, 710 03 Heraklion, Crete, Greece
[3]Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografrou, 15 771 Athens, Greece
[4]Department of Materials Science and Engineering, University of Crete, P.O. Box 2208, 710 03, Heraklion, Crete, Greece
Email: eglynos@iesl.forth.gr

Abstract:

The future of energy storage applications is related to the development of sustainable and "beyond Li-ion" battery chemistries. The desirable properties of such devices are accompanied by key features such as increased energy density, low manufacturing cost, and abundance of alkali metals. The latter is ideally suited to the use of sodium ions (Na+) due to their high abundance on the earth's crust, laying the groundwork for the development of battery technology based on materials with similar properties to those of Lithium ions. Here, we develop a fundamental understanding of the effect of cation chemistry on the structure - mechanical response - ion conductivity relationship in poly(ethylene oxide) (PEO)-based electrolytes. Various molecular weight of PEO were utilized and blended at various molar ration with lithium and sodium salts. Our data indicate that the Mw of the PEO, the cation size, and the strength of the cation-PEO interactions show a no trivial effect on the corresponding ion-conductivity and mechanical performance of these electrolytes at room temperature.

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High-Sensitivity Bimodal Plasmo-Photonic Refractive Index Sensor

D. V. Bellas[1,2,3], K. Fotiadis[2,3], E. Chatzianagnostou[2,3], D. Spasopoulos[2,3], S. Simos[2,3], L. Damakoudi[2,3], E. Lampadariou[1], O. Bhalerao[4,5], S. Suckow[4], A. L. Schall-Giesecke[4,5], M. Lemme[4,5], J-C. Weeber[6], P. Das[6], L. Markey[6], E. Lidorikis[1], and N. Pleros[2,3]

[1]Department of Materials Science and Engineering, University of Ioannina, 45110 Ioannina, GR
[2]Department of Informatics, Aristotle University of Thessaloniki, 54124 Thessaloniki, GR
[3]Center for Interdisciplinary Research and Innovation (CIRI-AUTH), 57001 Thessaloniki, GR
[4]AMO GmbH, Advanced Microelectronic Center Aachen, 52074 Aachen, Germany
[5]Electronic Devices, RWTH Aachen University, 52074 Aachen, Germany
[6]Laboratoire Interdisciplinaire Carnot de Bourgogne CNRS UMR 6303, Université de Bourgogne Franche-Comté, 21000 Dijon, France

Abstract: We present a new, ultracompact bimodal interferometric plasmonic sensor integrated on a SU-8 and/or SiN photonic waveguide platform. Two access photonic waveguides (SU-8 or SiN) are separated by an aluminum-based stripe, which resides on top of a thinner SU-8/SiN waveguide layer. In this way, two metal/insulator interfaces are formed at the top and bottom metal surfaces, which are capable of supporting two respective surface plasmon polariton (SPP) modes that are subsequently interfering with the output photonic waveguide. The upper metal surface is exposed to the surrounding medium and serves as the sensing element, while the lower surface serves as the reference branch of the interferometer. After a thorough optimization process, the device was fabricated and experimentally characterized. A clear bimodal interferometric response was obtained when the upper metallic surface was exposed to air and water, with both cases revealing an excellent agreement between the simulated and experimental values for the free spectral range. The experimental bulk refractive index sensitivity of the SU-8 based bimodal interferometer was evaluated by using water solutions on top of the upper metallic surface, demonstrating experimental sensitivity values of 4386 nm/RIU that are in good agreement with the value of 5806 nm/RIU expected from the simulation. The proposed sensing device takes advantage of the polymeric material SU-8 for the photonic waveguide, reducing in this way fabrication time and overall fabrication cost.

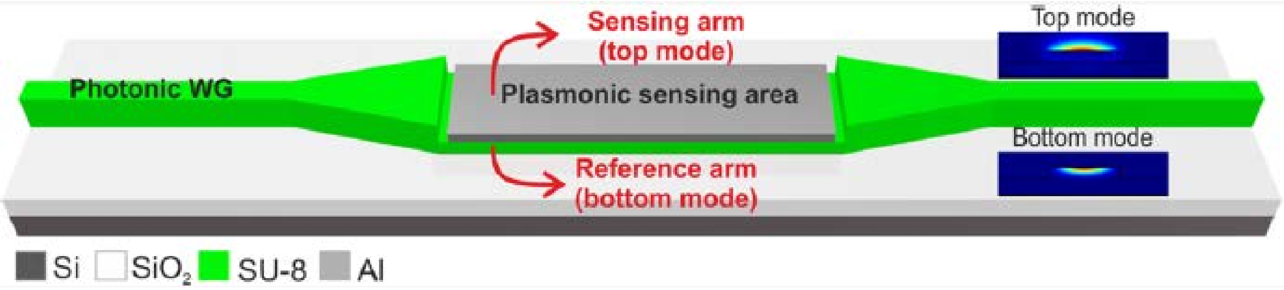

Fig. 1. Schematic of the SU-8 based Bimodal Plasmo-Photonic Refractive Index Sensor.