

**AAAFM**American Association for Advances in
Functional Materials

Materials For Life

UCLA 2021 August
18-20

Date: Wednesday, 18/Aug/2021

7:00am - 5:00pm	Registration: Registration
Theatre-Lobby	Location: Theatre-Lobby
7:10am - 7:20am	Opening Ceremony: Opening Ceremony
Theatre	Virtual location: Theatre
	Session Chair: Yu Huang
	Session Chair: Xiangfeng Duan
7:20am - 10:00am	Key-1: Keynote Session-1
Theatre	Virtual location: Theatre
	Session Chair: Yury Gogotsi
8:00am - 10:00am	FESC-1: Functional Materials for Energy Storage and Conversion Devices
AU 2410	Virtual location: AU 2410
	Session Chair: Weibin Chu
8:00am - 10:00am	FLNM-1: Fabrication of Low dimensional, Nano and 2D materials
AU 2412	Virtual location: AU 2412
	Session Chair: Pengpeng Zhang
10:00am - 10:20am	Coffee Break-1: Coffee Break
Theatre-Lobby	Location: Theatre-Lobby
10:20am - 12:00pm	Key-2: Keynote Session-2
Theatre	Virtual location: Theatre
	Session Chair: Yu Huang
10:20am - 12:00pm	FESC-2: Functional Materials for Energy Storage and Conversion Devices
AU 2410	Virtual location: AU 2410
	Session Chair: Haimei Zheng
10:20am - 12:30pm	FLNM-INV-1: Fabrication of Low dimensional, Nano and 2D materials
AU 2412	Virtual location: AU 2412
	Session Chair: Albert Wang
12:00pm - 1:00pm	Lunch-1: Lunch Break
Theatre-Lobby	Location: Theatre-Lobby
1:00pm - 3:00pm	EPMM-1: Electronic, Photonic and Magnetic Materials
AU 2410	Virtual location: AU 2410
	Session Chair: Wanli Yang
1:00pm - 3:00pm	FCM-1: Functional Composite Materials
AU 2412	Virtual location: AU 2412
	Session Chair: Donglei Fan
1:00pm - 3:00pm	Post-1: Poster Session
Theatre	Virtual location: Theatre
	Session Chair: Monish Chatterjee
3:00pm - 3:20pm	Coffee Break-2: Coffee Break
Theatre-Lobby	Location: Theatre-Lobby
3:20pm - 6:30pm	EPMM-2: Electronic, Photonic and Magnetic Materials
AU 2410	Virtual location: AU 2410
	Session Chair: Akshay Nagar
3:20pm - 6:30pm	FCM-2: Functional Composite Materials
AU 2412	Virtual location: AU 2412
	Session Chair: Liangbo Liang
3:20pm - 7:20pm	FESC-INV-1: Functional Materials for Energy Storage and Conversion Devices
Theatre	Virtual location: Theatre
	Session Chair: Elham Sahraei
	Session Chair: Muhammad Imran Shakir

Date: Thursday, 19/Aug/2021

8:00am - 8:10am	AAAFM-Awards: AAAFM-Award Ceremony
Theatre	Virtual location: Theatre
	Session Chair: Yu Huang
	Session Chair: Xiangfeng Duan
8:10am - 10:10am	AAAFM-Awards -1: AAAFM-Awards Presentations-1
Theatre	Virtual location: Theatre
	Session Chair: Xiangfeng Duan
8:10am - 10:00am	FESC-INV-2: Functional Materials for Energy Storage and Conversion Devices
AU 2410	Virtual location: AU 2410
	Session Chair: Elham Sahraei
8:10am - 10:00am	

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AU 2412	FLNM-INV-2: Fabrication of Low dimensional, Nano and 2D materials Virtual location: AU 2412 Session Chair: Rainer Timm
10:00am - 10:20am Theatre-Lobby	Coffee Break-3: Coffee Break Location: Theatre-Lobby
10:20am - 12:30pm AU 2410	FESC-3: Functional Materials for Energy Storage and Conversion Devices Virtual location: AU 2410 Session Chair: Miaofang Chi
10:20am - 12:30pm AU 2412	FLNM-2: Fabrication of Low dimensional, Nano and 2D materials Virtual location: AU 2412 Session Chair: Gerd Grau
10:30am - 12:30pm Theatre	AAAFM-Awards -2: AAAFM-Awards Presentations-2 Virtual location: Theatre Session Chair: Paul S. Weiss
12:00pm - 1:00pm Theatre-Lobby	Lunch-2: Lunch Break Location: Theatre-Lobby
1:00pm - 3:00pm AU 2410	EPMM-3: Electronic, Photonic and Magnetic Materials Virtual location: AU 2410 Session Chair: Lei Fang
1:00pm - 3:00pm AU 2412	FCM-3: Functional Composite Materials Virtual location: AU 2412 Session Chair: Swapnil B. Ambade
1:00pm - 3:00pm Theatre	Post-2: Poster Session Virtual location: Theatre Session Chair: KENAN SONG
3:00pm - 3:20pm Theatre-Lobby	Coffee Break-4: Coffee Break Location: Theatre-Lobby
3:20pm - 6:00pm AU 2412	FCM-4: Functional Composite Materials Virtual location: AU 2412 Session Chair: Xiaowu (Shirley) Tang
3:20pm - 6:40pm AU 2410	EPMM-4: Electronic, Photonic and Magnetic Materials Virtual location: AU 2410 Session Chair: Yang-Ki Hong
Date: Friday, 20/Aug/2021	
8:00am - 10:00am Theatre	Key-3: Keynote Session-3 Virtual location: Theatre Session Chair: Richard B. Kaner
8:00am - 10:00am AU 2410	EPMM-INV-1: Electronic, Photonic and Magnetic Materials Virtual location: AU 2410 Session Chair: Qibing Pei
8:00am - 10:00am AU 2412	EPMM-INV-2: Electronic, Photonic and Magnetic Materials Virtual location: AU 2412 Session Chair: Rizwan Raza Session Chair: Mohsin Ali Badshah
10:00am - 10:20am Theatre-Lobby	Coffee Break-5: Coffee Break Location: Theatre-Lobby
10:20am - 12:30pm AU 2410	EPMM-INV-3: Electronic, Photonic and Magnetic Materials Virtual location: AU 2410 Session Chair: Rainer Timm
10:20am - 12:30pm Theatre	FCM-INV-1: Functional Composite Materials Virtual location: Theatre Session Chair: Adam Weber
10:20am - 12:30pm AU 2412	FCM-INV-2: Functional Composite Materials Virtual location: AU 2412 Session Chair: Alexander Ayzner
12:00pm - 1:00pm Theatre-Lobby	Lunch-3: Lunch Break Location: Theatre-Lobby
1:00pm - 3:00pm Theatre	Post-3: Poster Session Virtual location: Theatre Session Chair: Umapada Pal
1:00pm - 3:30pm AU 2410	FCM-5: Functional Composite Materials Virtual location: AU 2410 Session Chair: Mohsin Ali Badshah

**1:00pm - 4:00pm**

AU 2412

EPMM-INV-4: Electronic, Photonic and Magnetic MaterialsVirtual location: **AU 2412**Session Chair: **Orion Ciftja**

Presentations

Key-1: Keynote Session-1

Time: Wednesday, 18/Aug/2021: 7:20am - 10:00am · Virtual location: Theatre

Session Chair: Yury Gogotsi

7:20am - 8:00am

Liquid metal 'putty-like' composites, and the path to, and making, F-Diamane

Rodney S. RuoffDepartments of Chemistry and Materials Science, School of Energy Science and Chemical Engineering Ulsan National Institute of Science & Technology (UNIST) Ulsan 689-798, Republic of Korea; ruofflab@gmail.com

We aim to discuss these topics:

(i) A liquid metal "plasticine" we invented by mixing gallium (or eutectics such as InGa, GaSn, GalnSn) with certain carbon fillers such as diamond particles, graphene oxide and reduced graphene oxide sheets, silicon carbide particles (Science Advances, 2021: doi.org/10.1126/sciadv.abe3767) hold promise as thermal interface materials (TIMS) and for EMI shielding, among other potential uses.

Then, I will cover a number of topics that were individually important, but were also a step-by-step route to achieving F-diamane, namely (ii) The large area single crystal metal foils (Cu, Ni, Co, Pd, Pt) we make by 'colossal grain growth' (Science, 2018: doi.org/10.1126/science.aao3373) allow (iii) growing "truly single layer and single crystal graphene" (no adlayers-no regions having 2 layers, 3 layers, etc.; Advanced Materials 2019: doi.org/10.1002/adma.201903615), (iv) obtaining large area, epitaxial, AB-stacked bilayer graphene on single crystal Cu/Ni(111) foils (Nature Nanotechnology: doi.org/10.1038/s41565-019-0622-8), and using this AB-stacked BLG to make (v) fluorinated single layer diamond ("F-diamane", Nature Nanotechnology: doi.org/10.1038/s41565-019-0582-z).

Time permitting, I will cover some or all of these topics as well: (vi) Why do wrinkles (and folds) appear in single layer graphene with some metal foil substrates and not others—it's the interplay between adhesion (friction) and deadhesion (Advanced Materials, 2018: doi.org/10.1002/adma.201706504, Advanced Materials 2019: doi.org/10.1002/adma.201903615; "fold-free single crystal graphene": submitted). The compressive strain we discovered in wrinkle-free (its epitaxial!) single layer graphene on the Cu(111) surface can (vii) 'drive' certain chemical reactions that do not occur for wrinkled and "not compressively strained" graphene regions (Advanced Materials, 2018: doi.org/10.1002/adma.201706504; and see more detail in Chemistry of Materials: doi.org/10.1021/acs.chemmater.9b01729). (viii) We invented a method to measure the intrinsic stiffness (that is, Young's modulus), and the fracture strength and toughness of centimeter-scale single layer graphene (Advanced Materials 2018: doi.org/10.1002/adma.201800888) and so we discuss the meaning of our measured values and of this method of measuring tensile-loading mechanics of macroscale ultrathin samples for future studies. We have (ix) folded an A5 sheet of ultrathin polycarbonate film that is 'laminated' to an A5-size sheet of single layer graphene 12 times (for fun!), and 10 times to generate samples whose mechanics we could explore by 3-point bending tests. Significant stiffening, strengthening, and toughening results from the graphene folds embedded in this composite sample that has 210 = 1024 layers of embedded graphene, and 1023 folds (Advanced Materials 2018: doi.org/10.1002/adma.201707449). Support from the Institute for Basic Science (IBS-R019-D1) is appreciated.

8:00am - 8:40am

Graphene and layered materials for photonics and optoelectronics

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Graphene and layered materials have great potential in photonics and optoelectronics, where the combination of their optical and electronic properties can be fully exploited, and the absence of a bandgap in graphene can be beneficial. The linear dispersion of the Dirac electrons in graphene enables ultra-wide-band tunability as well as gate controllable third-harmonic enhancement over an ultra-broad bandwidth, paving the way for electrically tuneable broadband frequency converters for optical communications and signal processing. Saturable absorption is observed as a consequence of Pauli blocking and can be exploited for mode-locking of a variety of ultrafast and broadband lasers. Graphene integrated photonics is a platform for wafer scale manufacturing of modulators, detectors and switches for next generation datacom and telecom. These functions can be achieved with graphene layers placed on top of optical waveguides, acting as passive light-guides, thus

simplifying the current technology. Heterostructures based on layers of atomic crystals have properties different from those of their individual constituents and of their three dimensional counterparts. The combinations of such crystals in stacks can be used to design the functionalities of such heterostructures, that can be exploited in novel light emitting devices, such as single photon emitters, and tuneable light emitting diodes.

8:40am - 9:20am

Atomically Precise Chemical, Physical, Electronic, and Spin Contacts

Paul S. Weiss

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Two seemingly conflicting trends in nanoscience and nanotechnology are our increasing ability to reach the limits of atomically precise structures and our growing understanding of the importance of heterogeneity in the structure and function of molecules and nanoscale assemblies [1]. By having developed the “eyes” to see, to record spectra, and to measure function at the nanoscale, we have been able to fabricate structures with precision as well as to understand the important and intrinsic heterogeneity of function found in these assemblies. The physical, electronic, mechanical, and chemical connections that materials make to one another and to the outside world are critical and are intertwined in terms of their function. Just as the properties and applications of conventional semiconductor devices depend on these contacts, so do nanomaterials, many nanoscale measurements, and devices of the future. We discuss the important roles that these contacts can play in preserving key transport and other properties. Initial nanoscale connections and measurements guide the path to future opportunities and challenges ahead. Band alignment and minimally disruptive connections are both targets and can be characterized in both experiment and theory [2]. Chiral assemblies can control the spin properties and thus transport at interfaces [3]. I discuss our initial forays into these areas in a number of materials systems.

Key Words: Nano, Materials, Band Alignment, Contacts, Spin

References

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9:20am - 10:00am

Exploring the Synthesis and Energy Storage Applications of Graphene

Richard B. Kaner

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Graphene is the ultimate two-dimensional material consisting of a single layer of sp² hybridized carbon. A facile, inexpensive, solid-state method for generating, patterning and electronic tuning of laser converted graphene will be discussed (Figure 1). Briefly, graphite can be converted into graphene oxide (GO) sheets, which readily disperse in water, and can then be reduced by various methods. Due to its unique ability to be solution processed and patterned, GO can be laser reduced to graphene directly onto various substrates without masks, templates, post processing, or transfer techniques. This work paves the way for the fabrication of inexpensive electrochemical energy storage devices that combine the energy density of batteries and the power density of capacitors.

Figure 1 (a) Schematic showing the fabrication process of a graphene micro-supercapacitor using a Light Scribe DVD drive. (b,c) This technique can create more than 100 micro-devices in a single run on virtually any substrate.

References:

1. D. Li, M.B. Muller, S. Gilje, R.B. Kaner and G.G. Wallace, “Processable aqueous dispersions of graphene nanosheets”, Nature Nanotechnology 3, 101-105 (2008).
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FESC-1: Functional Materials for Energy Storage and Conversion Devices

Time: Wednesday, 18/Aug/2021: 8:00am - 10:00am · Virtual location: AU 2410

Session Chair: Weibin Chu

8:00am - 8:10am

Water Photo-splitting for Hydrogen Generation using transition Metal Ion-or Lanthanide Ion-Doped Titanium dioxide Nanoparticle based Photon Up-conversion Materials

RAJAPAKSE MUDIYANSELAGE Gamini RAJAPAKSE¹, Asitha Udayanga Malikaramage¹, Gamaralage Rajanya Ashoka Kumara²

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Hydrogen is the cleanest and greenest fuel that can be used directly in internal combustion engine of motor vehicles and in fuel cells for cleaner and greener energy generation. However, hydrogen as hydrogen (H₂) molecules do not exist in the atmosphere. H₂ is abundant in the bound molecular forms: mainly as water and hydrocarbons. H₂ is mainly produced by petroleum cracking and the generated gas is used mainly onsite for production of petroleum-based chemicals and also for ammonia synthesis. H₂ is also produced by water electrolysis though the cost of production depends on cost of electricity. Honda and Fujishima first discovered photo-assisted electrochemical water splitting to H₂ and O₂, in 1972, using illuminated titanium dioxide electrodes. However, being a large band-gap semiconductor, TiO₂ absorbs in the UV region below 380 nm which is only present as 5% in the incident solar spectrum. Extensive research carried out since then enabled the development of efficient electron-hole separation to suppress their recombination. Deposition of noble metal (Pt or Pd) islands to catalyze H⁺ reduction and RuO₂ for hole capture for water oxidation are one such important strategies introduced. However, these catalysts lack the capability for utilization of full solar spectrum. In this research, novel strategy was developed where silver islands were deposited on TiO₂ nanoparticles for some visible light harvesting through their surface plasmon resonance effect and infrared upconverting electronic energy levels were introduced by doping TiO₂ with selected transition and lanthanide metal ions. A range of catalysts without and with Ag Islands [Ir(IV)-TiO₂, Eu(III)-TiO₂, Ho(III)-TiO₂, Nb(V)-TiO₂, Sm(III)-TiO₂, Ir(IV)-TiO₂, Cu(II)-TiO₂, Ir(IV)-TiO₂-Ag, Eu(III)-TiO₂-Ag, Ho(III)-TiO₂-Ag, Nb(V)-TiO₂-Ag, Sm(III)-TiO₂-Ag, Ir(IV)-TiO₂-Ag and Cu(II)-TiO₂-Ag] were synthesized and their infrared absorption verified by UV-Visible-NIR spectroscopy. Materials were duly characterized by powder XRD, XRF, FT-IR and SEM techniques. All these catalysts were shown to be more efficient in water photo-splitting when compared to that with bare TiO₂ and TiO₂ with only Ag Islands. However, in the absence of sacrificial hole-scavengers hydrogen and oxygen gases produced recombined generating excess heat that damaged the crystal lattice of the catalysts. Besides, when a gas mixture is generated its separation needs additional effort. As such, methanol and ethanol were used as sacrificial hole-scavengers to prevent oxygen generation. These catalysts generated hydrogen gas continuously when kept exposed to sunlight, in the stray light in the lab and also with upconverted infrared radiation when kept in the dark in the ambient laboratory conditions. Among these systems, Cu(II)-TiO₂-Ag, Nb(V)-TiO₂-Ag and Ir(IV)-TiO₂-Ag had the best performance of generating over 250 µl of H₂ gas per hour.

8:10am - 8:20am

Thermodynamic stability of La, Bi, and Sr ferrates : a hybrid DFT study

Eugene Heifets^{1,2}, Eugene A. Kotomin^{2,3}, Alexander Bagaturyants^{1,4}, Joachim Maier²

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Ferrates of Bi, La, and Sr are the end members of wide set of solid solutions (Bi_{1-x}Sr_xFeO_{3-δ}, Bi_{1-x}Sr_xFe_{1-y}CoyO_{3-δ}, and La_{1-x}Sr_xFe_{1-y}CoyO_{3-δ}). These materials are mixed ionic-electronic conductors and, therefore, have potential to be used or are already used for intermediate temperature cathodes of oxide fuel cells and related electrochemical and catalytic devices. In addition, BiFeO₃ perovskite attracts great attention due to its multiferroic properties. Also, SrFeO_{3-δ} has complex magnetic structure revealing colossal magnetoresistance effect what makes it interesting for spintronic applications; its properties strongly depend on oxygen non-stoichiometry. In this study ab initio hybrid functional approach was used for a study of thermodynamic stability of the considered ferrates with respect to their decompositions into binary oxides and to elements, as the function of temperature and oxygen pressure. The atomic (LCAO) basis sets were carefully re-optimized within the CRYSTAL computer code. Based on our calculations, the phase diagrams were constructed allowing us to predict the stability regions of BiFeO₃, LaFeO₃ and SrFeO_{3-δ} (δ=0, 0.125, 0.25, 0.5) in terms of atomic chemical potentials. This permits determining environmental conditions for existence of stable phases with the above-mentioned compositions. These conditions were presented as contour maps of oxygen atom chemical potential as a function of temperature and partial pressure of O₂ gas. A similar analysis was also performed using the experimental Gibbs energies of formation. The present modelling of SrFeO_{3-δ} strongly suggests a considerable attraction between oxygen vacancies. These vacancies are created during a series of above mentioned SrFeO_{3-δ} mutual transformations (δ=0→0.125→0.25→0.5) accompanied by oxygen release. It is shown that (within employed model) only the SrFeO_{2.5} phase appears to be stable in O₂-gas atmosphere.

Key Words: Ferrates, Fuel Cell Cathodes, Phase Diagrams, SOFC, Ab Initio Thermodynamics

References

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8:20am - 8:30am

Exploring the Flatland of 2D materials by Electrochemical STM: visualization of active sites in operando conditions

Stefano Agnoli¹, Tomasz Kosmala¹, Matthias Batzill², Gaetano Granozzi¹

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2D materials such as chemically modified graphenes, transition metal dichalcogenides, layered double hydroxide to name only a few, are having a huge impact on electrocatalysis providing materials with outstanding activity for a variety of reactions.[1]

However, despite the intense research efforts in this field, a clear identification of the real active sites in many reactions remains a great challenge, given the necessity to employ spatially and structurally sensitive techniques in operando conditions (i.e. during the application of an electrochemical potential in the presence of an electrolyte).

Here we present an innovative approach to the study of 2D materials by using electrochemical Scanning tunneling microscopy. As demonstrated by a seminal paper,[2] this technique allows identifying the presence of catalytic processes at the nanoscale by observing a typical noise in the tunneling current, which is due to instantaneous variations of the tunneling junction.

By using special model systems consisting of CVD grown transition metal dichalcogenides thin films (MoSe₂ and WSe₂), we achieved even atomic resolution during the hydrogen evolution reactions. This allowed us to distinguish the chemical activity of several chemical and morphological features such as single atom vacancies, step edges, and even exotic line defects such as metallic twin boundaries.[3]

References

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8:30am - 8:40am

Harvesting Up-converted Infrared Radiation for Dye-sensitized Solar Cells to Perform in the Dark

RAJAPAKSE MUDIYANSELAGE GAMINI RAJAPAKSE¹, Asitha Udayanga Malikaramage¹, Gamaralage Rajanya Ashoka Kumara²

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Solar spectrum incident on the Earth surface consists mainly of 5% ultraviolet, 40-45% visible and 50-55% infrared radiation. However, dye-sensitized solar cells (DSCs) only utilize UV and some visible components but not the major IR fraction since IR is incapable of electronic excitation. In order to utilize IR radiation, these IR photons have to be added to get UV or visible radiation via the process known as photon up-conversion. Photon up-converting crystals based on NaYF₄ doped with Er(III) or Yb(III) and both Er(III) and Yb(III) are used in bio-imaging since IR radiation has deeper penetration when compared to that of UV and visible and the detection is from colors generated in the visible range. For the first time, these up-converting lanthanide crystals were used together with N-719 dye to coat interconnected nanoparticles of TiO₂ with them to be used in both liquid electrolyte (I-/I³⁻ in acetonitrile)-based and in all DSCs. The presence of lanthanide crystals on TiO₂ particles is proven by XRF measurements and its ability to absorb in near IR by UV-visible-NIR spectroscopy. Although liquid-type DSCs did not perform with infrared illumination in the dark, the all solid-state solar cell gives appreciable efficiency of 4.5% with 1 Sun illumination (UV-Visible-NIR) and 0.4% efficiency only with NIR illumination, in the dark, despite the fact that the intensity of NIR source used is much less than 1 Sun. The performance of the liquid electrolyte-based DSC is inferior to one without up-conversion crystals even with 1 Sun illumination and it did not give any efficiency with infrared illumination alone. This is mainly due to evaporation of the volatile solvent and consequent drying up of the DSC. A 4.5% efficiency for a all solid-state DSC is perhaps the highest so far recorded. The fact that it works only with IR radiation indicates that solar cells can be fabricated to work even in the night. This is an entirely new concept and this research gives evidence for the proof of concept.

References

A.U. Malikaramage, G.R.A. Kumara and R.M.G. Rajapakse*, A manuscript aiming at Science is in preparation.

8:40am - 8:50am

Structural, Electrochemical and Optical Properties of Small Organic Molecules for Solar Cell Applications

Phuong-Truc Pham, Mamoun M. Bader

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We developed synthetic strategies to design a variety of donor/acceptor molecules based on triphenyl amines, oligothiophenes, oligoethylenedioxy thiophenes and ladder type fused heterocyclic oligomers endowed with strong acceptor moieties incorporating tricyanovinyl-, dicyanovinyl-, halogens, and TCNQ- like groups. The single crystal structural analyses of a wide range of closely related molecules offer insights into the role of various groups in driving the observed packing motifs. Furthermore, we used cyclic voltammetry to characterize the electron donating and accepting abilities of these materials in solution and to provide insights into the evolution of the relative HOMO-LUMO levels as a function of introduction of specific substituents. We also carried out optical characterization of these materials with emphasis on fluorescence and solvatochromic behavior as a function of structural modification. By systematically tailoring the molecular structure we monitored how optical and electrical properties evolve. Finally, we use the shifts in CN stretching frequencies in these materials as a possible feature to render them useful as biological markers.

8:50am - 9:05am

In-situ Study of Electrode Electrolyte Interface Phenomena Using Liquid Cell Electron Microscopy

Haimei Zheng

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We study alkali metal (e.g., Li and Na) plating and stripping in situ using liquid cell transmission electron microscopy (TEM)¹⁻³. As a passivation interfacial film formed from the reduction of the electrolyte, solid-electrolyte interphase (SEI) plays an important role in the cycle stability of Li-ion batteries. Many efforts have been devoted to an understanding of the nature of SEI through various microscopy and spectroscopic approaches, including in situ x-ray scattering, and neutron reflectometry. In situ observations are beneficial as it avoids complications due to sample exposure to air and moisture. In situ liquid cell TEM imaging with nanoscale chemical analysis complements these studies. Liquid phase TEM observations and nanobeam diffraction of SEI on the electrode revealed that the SEI layer contained LiF nanocrystals distributed in an amorphous matrix,¹ in contrast to the previous understanding of a denser layer of inorganic components adhering to the electrode with a porous organic outer layer exposing to electrolyte. Further advances of electrochemical liquid cell TEM allowed the mapping of spatially resolved SEI chemistry on individual lithium nanograins.² The observation revealed that Li dendrites can be suppressed by a cationic polymer coating on the electrode, thus uncovering a potential path to Li dendrite suppression.

9:05am - 9:15am

Phase transitions of EMIM TFSI ionic liquids (1-Ethyl-3-methylimidazolium bis (trifluoromethylsulfonyl) imide confined in nanocarbons

Malgorzata Sliwinska-Bartkowiak¹, Konrad Rotnicki¹, Monika Jazdzewska¹, Anatolii Beskrovnyi²

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Currently, a much research in electrochemistry is concerned with the effect of direct application of the ionic liquids as electrolytes for supercapacitors (SC) – the energy storage devices operating through the formation of an electrical double-layer, by simple separation of ions at the electrode/electrolyte interface. The high applicability of these systems results from their exceptionally fast charging/discharging time measured in few seconds. Due to the fact the operation conditions for SC require low temperatures, an important issue is an investigation of melting behavior of ionic liquid applied as an electrolyte.

We report the experimental studies of the melting behavior of 1 - Ethyl -3 - methylimidazolium bis(trifluoromethylsulfonyl)imide (EMIM TFSI); for this purpose the methods of dielectric spectroscopy (DS) and differential scanning calorimetry (DSC) in wide temperature ranges were applied. To investigate the structural properties of the system the temperature-controlled WAXS and Neutron Diffraction methods were adopted. The measurements of the complex permittivity of the studied EMIM TFSI allowed us to determine the relaxation of the system in wide temperature range from 140 K to 300 K. The results obtained from DSC and DS indicate that the ionic liquid on the heating process undergoes two phase transitions: solid-solid transition at temperature 230 K and the melting transition at 257 K, wherein the melting process is not homogeneous. Based on the structural studies results, performed in the temperatures range 10 K – RT, it was shown that in the temperature range 10 K-230 K EMIM TFSI forms a crystal monoclinic structure where the rotation motions of molecular groups are observed. At the higher temperature up to the melting temperature the crystal structure is undefined and the rotational motions of molecular groups are changed. The similar studies performed for EMIM TFSI confined in carbon micropores show that the melting process of IL in pores is unhomogeneous and melting temperature of IL decrease relatively to EMIM TFSI bulk melting point.[3]

Key Words: Ionic Liquids, Melting Transition, Nanocarbons, Energy Storage

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Financial support for the NCN grant No UMO-2016/ 22/A/ST4/00092 is gratefully acknowledged

9:15am - 9:25am

Real-space topological ferroelectricity and self-epitaxial hetero-nanolayers in nickel phosphides

Xiankui Wei¹, Gustav Bihlmayer², Yuri V. Kolen'ko³, Lifeng Liu³, Stefan Blügel², Joachim Mayer^{1,4}, Rafal E. Dunin-Borkowski¹

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Surface compositional, atomic and electronic structures play key roles in controlling activity of catalysts during electrochemical reactions. As for the supporting matrix, factors such as conductivity, elemental valence state, polyhedral polarity and spin structure [1-3] are also important in influencing performance of the catalysts. However, for earth-abundant and efficient transition-metal phosphides used for water splitting, such atomic-scale structural information is largely missing, which hinders design and optimization of catalysts with superior electrochemical activity. Here, we report the discovery of real-space topological ferroelectricity in non-

centrosymmetric Ni₂P (space group P-62m). Focusing on polyhedral polarity [4], we establish symmetry equations of polarity and the solution yields that the polarity couples with elemental valence states through nickel atomic sites, which is verified by valence state measurement using electron energy-loss spectroscopy (EELS) and structural characterization. First principles calculations reveal that associated with center-convergent to center-divergent transition of topological geometry under in-plane compressive strain (winding number $n = 1$), the polyhedral polarity also couples to momentum-dependent spin polarization. The dual roles of nickel cations, i.e., their polar displacements and 3D bonding network, enables the coexisting topological polarity with metallicity [5]. In combination with electron-beam bombardment, our image-simulation-based scanning transmission electron microscopy (S/TEM) study reveals coverage of self-epitaxial Ni₂P and NiP_x ($0 < x < 0.5$) nanolayers on (001) surfaces of Ni₅P₄ nanosheets [6]. The discovery of topological ferroelectricity and core-shell scenario in nickel phosphides provide novel insights to understand the catalytic performance of transition-metal catalysts for electrochemical energy conversion.

Key Words: Water splitting, Nickel phosphide, Topological ferroelectricity, Core-shell

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9:25am - 9:40am

Materials and Molecular Modeling, Imaging, Informatics and Integration (M3I3)

Seungbum Hong^{1,2}, Jong Min Yuk¹, Hye Ryung Byon³, EunAe Cho¹

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M3I3 is an algorithm to perform a reverse engineering of future materials. Fast followers usually copy the first movers' products by reverse engineering them. For example, in case of the state-of-the-art battery products, the competitors dissect them into pieces and analyze the structure and composition of each part such as cathode, anode, electrolyte and separator. This so called "reverse engineering" is the cheapest way to catch up with the forefront runners in the ever-expanding competing world. For the front-runners, they also need a way to defend themselves and aggressively keep the distance from their competitors, and that's why they invest a huge amount of resources into research and development of new materials, devices, systems and platforms, and file patents all over the world. M3I3 provides a means to achieve this goal effectively by mimicking "reverse engineering" strategy with a higher level of creativity. M3I3 reverse engineers future materials of interest with superior performance and reliability as well as with minimum cost and environmental impact.

How is this possible? Reverse engineering starts from analyzing the structure and composition of the cutting-edge materials or products. Once we determine the performance of our targeted future materials, we need to know the candidate structure and composition of the future materials. This knowledge can only be available if we know the structure-property or the property-structure relationship of all materials and molecules at all scales. High-quality multi-scale and multi-dimensional experimental data will be the key to the success of our approach. But there are critical challenges such as collecting and analyzing those data with consistency.

We hope to address those challenges during the workshop and form a clearer idea for our future direction.

Key Words: M3I3, Materials Imaging, Machine Learning, Data Mining, Structure-Property, Processing-Structure

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9:40am - 9:50am

Structure from Darkness: Exploring Ionomer interactions in Fuel-Cell Inks and Resultant Performance Impacts

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The fabrication of proton-exchange-membrane fuel-cell catalyst layers is traditionally an empirically based black art. These layers are typically fabricated from multicomponent inks composed of Pt/C nanoparticles, a dispersion of ion-conducting polymer or ionomer, and all in an alcohol/water mixed solvent system. These inks are then coated onto ionomer membrane or gas-diffusion layers using different techniques such as ultrasonic spray and then allowed to dry to form a triple percolated pathway for gas, ions, and electrons to transport and react at the catalyst sites. Thus, the interactions within the ink control the catalyst-layer structure and resultant performance. In this talk, we will explore the underlying interactions of the constitutive components of the fuel-cell inks, with a focus on how the ionomer and catalyst interact. Such studies include isothermal titration calorimetry, dynamic light scattering, zeta potential

measurements, and quartz crystal microbalance. These studies will be complemented by in-situ characterization of fuel-cell performance and limiting current analysis for different ionomers. The findings demonstrate the key roles that ionomer content and identity play in interacting through hydrophobic forces with the particle surface and controlling catalyst-layer structure and performance. It will be shown that higher ion-exchange polymers result in larger interfacial interactions but lower local transport resistances. The studies provide insights into catalyst-layer fabrication and point to future material design trends and targets for these functional composite materials.

9:50am - 10:05am Warning: This presentation lies outside the session time!

Hybrid Smart Textiles and Devices for Energy Harvesting & Storage: Nanotechnology in Motion towards Self-Powered Technologies

Clara Pereira¹, André M. Pereira², Rui S. Costa^{1,2}, Joana S. Teixeira^{1,2}, Ana L. Pires²

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The ever-growing progress of the emerging market of wearable electronics has been driving the need for advanced all-in-one energy harvesting & storage technologies integrated on clothing for several applications ranging from Healthcare and Sports to Fashion and Defense. Thermoelectric energy harvesting technology is a promising solution for wearables since it convert the low-grade waste heat from ubiquitous thermal energy sources into electrical energy. Supercapacitors are a clean and safe energy storage solution to produce wearable energy storage clothing, owing to their high power density, fast charging, long cycle life and robustness.

The combination of both technologies in a single ALL-IN-ONE device opens new horizons towards the next generation of self-powered flexible/wearable electronics.¹

Nanotechnology and Nanomaterials fostered innovation in the Textile and Clothing industry, to impart new functionalities on fabrics while preserving their comfort and lightness properties.

In this talk, we will provide an overview of our recent achievements in the design of smart textiles and devices for energy applications, from supercapacitor devices towards an innovative all-in-one self-powered energy harvesting & storage technology.²⁻⁴ The journey from the concept and design of advanced functional nanomaterials, their incorporation on textile and flexible plastic substrates and assemble of hybrid multi-tasking systems will be presented.

Key Words: Hybrid Nanomaterials, Smart Textiles & Devices, Energy Storage, Energy Harvesting

Acknowledgments: This research was funded by FEDER through COMPETE 2020-POCI and by Fundação para a Ciência e a Tecnologia (FCT)/MCTES under Program PT2020 in the framework of the project PTDC/CTM-TEX/31271/2017. This work was also supported by UIDB/50006/2020 and UIDB/04968/2020 with funding from FCT/MCTES through national funds. CP and JST thank FCT for FCT Investigator contract IF/01080/2015 and PhD scholarship with reference SFRH/BD/145513/2019, respectively.

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FLNM-1: Fabrication of Low dimensional, Nano and 2D materials

Time: Wednesday, 18/Aug/2021: 8:00am - 10:00am · Virtual location: AU 2412

Session Chair: Pengpeng Zhang

8:00am - 8:10am

Homogeneity Region of Palladium (II) Oxide Nanocrystalline Films for Gas Sensors

Goran Karapetrov¹, Alexander Samoylov², Dmitry Pelipenko², Olga Chuvenkova³, Sergey Ivkov³, Sergey Turishchev³

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Low level ozone which is a product of industrial activity, transportation, etc., has been accumulating at the surface of the Earth during the last twenty five years. WHO and US EPA declared that ozone O₃ and nitrogen dioxide NO₂ could be very dangerous for human health especially for children, the elderly, and patients with lung diseases [1]. Pollution of ambient air with low level O₃ and NO₂ is a serious problem owing to cyclic processes of these gases via mutual transformation under sunlight [2]. Interaction of O₃ and NO₂ with volatile hydrocarbons produces many toxic organic substances as a result of oxidation reactions. Palladium (II) oxide nanostructures were employed for O₃ and NO₂ detection. Homogeneous nanocrystalline PdO films (with thicknesses ranging around 10, 35, and 100 nm) with p-type conductivity and energy band gap $E_g \sim 2.3$ eV were prepared on polished poly-Al₂O₃, SiO₂/Si (100), optical quality quartz, and amorphous carbon/KCl substrates by deposition of pure Pd metal layer and subsequent thermal oxidation in oxygen atmosphere at temperatures $T = 620 - 1070$ K. It was established that nanocrystalline PdO films have the high sensitivity, operation speed, stability, short recovery time, and good reproducibility of sensor response [3, 4]. In this work by XPS measurements it has been found that PdO nanocrystalline films contain a small concentration of palladium atoms in oxidation state (+4). The composition of PdO films within the homogeneity region is one of key parameters which determine the sensitivity toward the toxic gases with the oxidative and reductive properties [2]. The precise XRD experiments have shown that the lattice constants of the tetragonal crystal structure of homogeneous nanocrystalline PdO films increase with the rise of oxidation temperature up to $T = 1020$ K. On the basis of the unit cell volume values of PdO films prepared at temperatures between $T = 620 - 1070$ K and well known values of Pd (2+), Pd (4+), and O (2+) ionic radii the width of homogeneity region has been calculated. It has been found that nanocrystalline PdO films have excess of oxygen atoms from the stoichiometric ratio.

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8:10am - 8:20am

Design of water-soluble fullerene derivatives with promising antiviral properties

Olga A. Kraevaya¹, Alexander S. Peregodov², Alexander F. Shestakov^{1,3}, Dominique Schols⁴, Pavel A. Troshin¹

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Viral infections are responsible for 90% of human infectious pathologies. Efficiency of the existing antiviral drugs is limited by their narrow action spectra, development of drug-resistant viral strains and toxicity effects. Therefore, there is an urgent need for the development of new types of antivirals with improved performance. Water-soluble fullerene derivatives demonstrated extremely promising antiviral properties against HIV, CMV, HSV, Hepatitis C, Influenza, and Stomatitis and Ebola viruses in some cases overcoming efficiency of commercial drugs. Importantly, several fullerene derivatives inhibit simultaneously more than one viral target, thus suppressing significantly the formation of drug resistance.

Recently we reported efficient and selective methods for the synthesis of a broad range of water-soluble fullerene derivatives [1-3], which substantially decreased costs of these compounds and made them available in bulk quantities for biological studies. We will discuss four new synthetic routes for conversion of readily available C₆₀Cl₆ and C₇₀Cl₈ precursors to a variety of stable water-soluble fullerene derivatives bearing up to 16 carboxylic groups in their molecular frameworks. Several fullerene derivatives revealed low toxicity in combination with a pronounced activity against Influenza, HIV, CMV, and HSV, which makes them promising compounds for the development of novel antiviral drugs.

Key Words: Water-Soluble Fullerene Derivatives, Antiviral Properties

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8:20am - 8:30am

Permethylated two-dimensional Metal-Organic Frameworks - Promising Candidates for Emerging 2D Materials

Alexandru Constantin Stoica, Madalin Damoc, George T Stiubianu, Maria Cazacu

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After the discovery of graphene with the set of properties that essentially distinguish it from other carbon allotropes, ultra-thin layered materials, classified as 2D nanomaterials, enjoy growing interest due to their unique properties [1]. In this context, although three-dimensional metal-organic frameworks (3D MOFs) are currently studied for addressing challenges concerning energy and environment, recently two-dimensional MOFs have become of interest from the perspective of their approach as 2D materials. The possibilities of variation of their construction units (metal and ligand) allow the fine control of the material properties. But during the forming process, the 2D layers are stacked by intermolecular interactions, leading to materials with increased dimensions. To study specific properties of 2D material, it must be delaminated and isolated as individual layers with a thickness/surface ratio as small as possible, which is a challenge. Both the top-down and bottom-up approached strategies proved to be quite difficult involving large consumption of time, materials, energy, etc., without guaranteeing the stability of the individual layers.

A promising alternative pathway is the design and synthesis based on suitable precursors of two-dimensional metal-organic networks with extremely weak intermolecular interactions, which facilitate delamination in nanosheets [2,3]. Our original approach consists in the use of ligands containing permethylated silicone units, which by their natural exposure and low surface tension shield the 2D structure and prevent the establishment of quantifiable interactions among neighboring layers. Binary mixtures of ligands with a dicarboxylic acid with tetramethyldisiloxane spacer and different bipyridyl derivatives for different metal ions (Co, Zn, Mn, Cd) were used successfully. The obtained structures were evaluated in terms of structure, size, morphology and properties (thermal, magnetic, electrical, optical). Preliminary assessments have been made regarding the ability to respond to external stimuli. Acknowledgements: This work was supported by a grant of Ministry of Research and Innovation, CNCS - UEFISCDI, project number PN-III-P4-ID-PCE-2020-2000 (2D-PerMONSIl), within PNCDI III, Contract 207/2021.

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8:30am - 8:40am

Meso-Entropy Materials: From PAH Isomers to Topological Defect of Graphene

Xiaodong Zhuang

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In the past decades, various materials have been developed, especially for carbon-rich materials. The most popular carbon-rich materials include fullerene, carbon nanotube, graphene, graphite, diamond, and polycyclic aromatic hydrocarbons (PAHs). Although studies appear to be exhaustive, the relationship between these materials remains unclear. Even for one of them, the understanding at chemistry level is still at the stage of hybridization difference. In this talk, I'd like to propose a new method, the meso-entropy concept, to re-understand carbon materials and forecast new carbon-rich materials with new properties.

8:40am - 8:50am

Ultrafast Acoustofluidic Exfoliation and Manipulation of Transition Metal Dichalcogenide Crystals

Amgad Rezk, Heba Ahmed, Kourosh Kalantar-Zadeh, Leslie Yeo

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2D crystalline materials possess outstanding performance for application in electronics, energy and catalysis, however, their realization pivots on the ability to exfoliate them from a 3D bulk down to monolayers. However, this goal remains elusive particularly in terms of a rapid processing method that facilitates high yield and control over the material dimensions, while preserving high crystal quality. In this talk, we uncover an ultrafast exfoliation mechanism that exploits the piezoelectric nature of a number of these materials and that involves triggering electrically induced mechanical failure across the weak domains of the material. In particular, we demonstrate that microfluidic nebulisation using high frequency acoustic waves exposes a bulk 3D crystalline piezoelectric material such as molybdenum disulphide (MoS₂) and tungsten disulphide (WS₂) to a combination of a large mechanical and electrical fields. These large mechanical accelerations exceeding 108 m/s² and applied electric fields surpassing 108 V/m rapidly cleave the materials into nanosheets comprising mainly single layers, thus constituting a continuous method, with high-throughput yet on a miniaturised chip-scale that opens new possibilities for scalable production and spray coating. In addition, these acoustic waves are shown to modify the Photoluminescence and bandgap properties of single as well as odd layered MoS₂.

8:50am - 9:00am

Observation of Layer Thinning in Exfoliated Tellurene via Oxygen Annealing: Towards Few Layers Tellurene

Ghadeer Aljalham¹, Sarah Alsaggaf¹, Khalid Alhamdan¹, Sarah Alodan^{1,2}, Abrar Alhazmi^{1,3}, Olaiyan Alolaiyan¹, Shahad Albawardi¹, Moh. R. Amer^{1,4}

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Tellurene (Te) has become the focus in 2D materials due to its tunable bandgap, anisotropic behavior, and resilience to ambient conditions.[1] Nonetheless, Te flake exfoliation is challenging and suffers from low yield due to its crystal structure and layer to layer bonding. Consequently, fabrication of a few layers of Te is limited to epitaxial growth or liquid exfoliation.[2,3] In this work, we report a thermal annealing technique conducted in a controlled oxygen environment applied to mechanically exfoliated Tellurene. According to our AFM measurements, a significant decrease in thickness is observed for Te nanosheets from bulk (~1µm) to few layers (~25nm). This thinning has been confirmed using Raman spectroscopy, where a clear blue shift measured for A1 and E2 Raman modes after thermal annealing. We observe a favorable thinning direction for all thinned Te nanosheets, which is attributed to the anisotropy behavior of these Te nanosheets. Our results shed some light on a simple annealing technique for future Te device applications.

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9:00am - 9:10am

A theoretical study of changes in the electronic properties of ZSM-5 zeolite under the transition from bulk 3D to lamellar 2D structure

Joel Antúnez-García, D. H. Galván, Vitalii Petranovskii, Rosario I. Yocupicio-Gaxiola, Fabian N. Murrieta-Rico, Sergio Fuentes

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As the world's population is continuously growing, the demand for energy, food, and healthcare resources is constantly increasing. In this regard, the challenge facing science and technology is to develop processes for producing sustainable chemicals with low impact on the planet's biosphere. Zeolites are materials that have already shown a significant role in a large number of sustainable processes and even today they continue to represent great innovations. Currently, the latest technology uses nanostructured zeolitic materials, which leads to an improvement in the properties that its analogous represents in bulk. Potential applications of these new materials are in the areas of renewable energy, catalysis, agri-food sector, environmental improvement, sensors, etc [1,2]. Improving the diffusion of molecules within zeolites could boost the catalytic processes that they offer. Particularly, improving the diffusion of molecules within zeolites could increase the catalytic processes that occur in them. This can be achieved in zeolite by reducing its size to the order of nanometers, or by creating flat 2D structures. Although there is no physical obstacle that restricts the production of lamellar zeolites with a nanometric thicknesses, only some of them have been possible to synthesize experimentally, and one of them is known as ZSM-5 [3]. To gain understanding about how the properties of ZSM-5 zeolite are modified when one dimension is reduced to a nanometer size (laminar zeolites), DFT theoretical computations were performed. For the appropriate contrast, the ZSM-5 matrix of purely silica and with an aluminum atom isomorphically substituted in the unit cell were considered for both the bulk and lamellar cases. Additionally, both Na⁺ and H⁺ were examined as the exchange cations. The results show that, in contrast to its bulk counterpart, and regardless of the nature of the exchange cation, the conduction band gap for the laminar ZSM-5 zeolite tends to zero. On terms of a population analysis, the acidic/basic character of distinct atoms in various configurations was evaluated. From this analysis, it was found that the acidic/basic character for lamellar zeolite represents an improvement over the respective bulk counterpart.

9:10am - 9:25am

Theory of electronic and optical properties of pristine and defective graphene quantum dots

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Graphene quantum dots (GQDs) are 0D carbon-based materials that exhibit several striking characteristics of graphene combined with a tunable bandgap due to quantum confinement effects. The tailoring of the optical bandgap of GQDs can be achieved by varying their shape, size and also by introducing topological anomalies like Stone-Wales (SW) defects. In order to realize the full potential of pristine and defective graphene nanostructures in optoelectronic applications, it is essential to obtain a deep understanding of their electronic structure and optical properties. In this talk, we will discuss the theory of electronic structure and optical properties of these GQDs, within a Pariser-Parr-Pople (PPP) model Hamiltonian-based correlated electron approach, developed in our group. We will present results of theoretical calculations of the optical absorption spectra of pristine as well defective GQDs of different shapes and sizes. Our calculations have revealed that the absorption spectra are redshifted with the increasing sizes of quantum dots. Our studies also demonstrate that SW type reconstruction is responsible for the appearance of new defect-induced peaks below the optical gap and dramatically modifies the optical absorption profile. In addition, our investigations signify that electron correlation effects become more dominant for SW-defected GQDs. We finally establish that the introduction of SW defects at specific locations strongly enhances

light absorption in the visible range, which is of prime importance for designing light-harvesting, photocatalytic, and optoelectronic devices.

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9:25am - 9:35am

Spectroscopic and Structural Properties of Atomically Thin Yb³⁺-doped MoS₂ films, deposited using near-IR femtosecond pulsed laser source

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The physics of two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides (TMDs) have been investigated for a range of optoelectronic device applications [1]. Tuneability of bandgap and control of photoluminescence wavelength in 2D materials are important features for demonstrating applications in energy conversion, light emission, and spintronic devices [2]. Recently, the 2D layered materials grown by pulsed laser deposition technique have attracted attention for integrated optoelectronics [3].

In this presentation, we report femtosecond pulsed laser deposition of undoped and rare-earth Yb³⁺-ion doped MoS₂ films. The femtosecond laser with a wavelength of 800 nm, a pulse duration of 100 fs and a repetition rate of 1 kHz were used to deposit the layered MoS₂ films. Different deposition parameters were used to form few nano meter thick layered structures of MoS₂ films. For achieving such a control of film thickness over 1cm² deposition area, the laser fluence at 3 J/cm², Ar pressure of 10 mTorr and substrate temperature at 500°C were maintained. The deposited films were characterized by Raman spectroscopy which clearly showed the characteristic of A_{1g} and E_{2g} modes. The separation between the two Raman modes is 23 cm⁻¹, which translates it into the 4-6 number of layers. In Yb³⁺-ion doped MoS₂ films, the Raman modes were shifted to higher frequencies, implying the possible effect of Yb³⁺ doping and/or defects on 2D MoS₂ structure. A further confirmation of the number of layers formed and doping were verified using transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS). Nonlinear optical properties of undoped and doped MoS₂ films were studied using open aperture Z-scan technique. For Z-scan, 7 ns pulses from the second harmonics of the Nd-YAG laser centered at 532 nm with a repetition rate of 10 Hz were used to excite the sample. In Yb³⁺-doped films, enhancement in saturable absorption (SA) at room temperature was observed, which is particularly advantageous for applications in nano-photonics devices such as passive modelocking and optical switches. Our results provide important fundamental insight into the nonlinear optical response and are of crucial importance in designing novel multifunctional rare-earth doped 2D materials.

Key Words: MoS₂, RE-ion dopant, Photoluminescence, Optical Nonlinearity

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9:35am - 9:50am

Functionalization of Exposed-Core Fibers with CVD-Grown Monolayer Transition Metal Dichalcogenides: Photoluminescence and Nonlinearity

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Monolayer transition-metal dichalcogenides [1] (TMDs) are a new and highly interesting material for optics and photonics due to their rich photophysics, their strong interaction with light, and large optical nonlinearities [2]. However, their usage in photonic applications is limited by the sub-nanometer interaction length, imposed by their atomic thickness; the enhancement of which is essential for future applications. Possible use-cases are also hampered by the difficulties in transferring monolayer crystals onto photonic circuitry, such as waveguides or optical fibers.

Recently, we have demonstrated a novel type of scalable functionalization technique for exposed-cored optical fibers (ECF) [3], where MoS₂ and WS₂ crystals are directly grown on the fiber's core. The growth is based on a one-pot chemical vapour deposition CVD process and leads to high quality monolayers crystals being grown directly on the core of the ECFs and in physical contact with the evanescent field of the fiber's guided mode. We show that by adjusting the growing condition, the density of TMDs monolayers can be tuned.

The TMDs interact with the guided light by the evanescent field of the ECF's guided mode, leading to exciton formation, photoluminescence (PL) emission, and enhanced nonlinear interaction, which can be excited through and detected by light being guided in the ECF. The incident light was launched into one facet of the fiber and the PL or nonlinearity generated light was collected

from the other face. We observe guided-wave exciton emission at 678 nm and 622 nm for MoS₂ and WS₂, as well as enhanced third harmonic generation. Other forms of enhanced nonlinear effects will be discussed in the presentation, as well. We expect that our work opens new perspectives for TMD-based active, guided wave photonic circuits.

9:50am - 10:00am

Chemistry of 2D monoelements beyond graphene

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Monoelemental two-dimensional (2D) materials are at the forefront of current material research. Beyond graphene, the large family of unexplored materials remain unexplored. The development of these materials starts rapidly in last few years. In the carbon or so called tetrel group are beyond carbon silicon, germanium and tin. These elements are capable to form a layered allotrope, however the synthesis methods are not so straightforward as for the graphite. All these materials are non-zero band-gap semiconductors with huge application potential in electronic and optoelectronic devices. This property opens new application possibilities in electronic and optoelectronic devices. Also, the research in the field of energy storage and conversion, as well as sensors and other fields, is rapidly growing. The properties strongly correlate with chemical modifications and functionalization. Compare to graphene, the chemistry of its heavier counterparts remains significantly less explored.¹

The main route for top-down methods of synthesis are based on exfoliation and functionalization of Zintl phases with general formula AB₂ consisting from hexagonally arranged Si/Ge layers separated by alkaline earth atoms, typically calcium. The exfoliation procedure is typically based on reaction with acid at low temperature forming hydrogen terminated surface. In this contribution will be demonstrated novel methods and strategies in synthesis and functionalization of silicene and germanene monolayers. The methods providing controlled functionalization surfaces are based on formation of negatively charged silicene/germanene and subsequent reactions with halogen derivatives, formation of reactive halogenated intermediates or direct reactions of Zintl phases with bromine or iodine derivatives. The developed methods were used for introduction of various alkyl and aryl derivatives in order to control transport and optical properties of functionalized materials. The functionalized germanium derivatives exhibit strong photoluminescence, which maxima can be tuned by substitution with various alkyl and aryl derivatives. For newly developed materials were utilized various applications including gas sensors, hybrid organic-inorganic OLED devices and photocatalytic water splitting.

10:00am - 10:10am Warning: This presentation lies outside the session time!

Oxidation and stabilization of 2D MXene nanosheets

Xiaofei Zhao, Touseef Habib, Aniruddh Vashisth, Jodie Lutkenhaus, Miladin Radovic, Micah Green

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MXenes, such as Ti₃C₂T_x, are fascinating 2D nanomaterials with an attractive combination of functional properties suitable for applications such as batteries, supercapacitors, and strain sensors. However, practical uses of MXenes, such as Ti₃C₂T_x, remains challenging as these nanosheets are known to oxidize and degrade quickly from reacting with water and dissolved oxygen. Here, we examine oxidation of MXene nanosheets in various media (air, liquid, and solid) via multiple types of measurements to assess their shelf stability. The oxidation rate of MXene nanosheets were observed fastest in liquid media and slowest in solid media and can be accelerated by exposure to UV light. We also demonstrate an effective method to retard the oxidation of colloidal Ti₃C₂T_x MXene nanosheets by introducing antioxidants such as sodium L-ascorbate. The success of the method is evident in the conductivity and colloidal stability of Ti₃C₂T_x. Even in the presence of water and oxygen, the electrical conductivity of Ti₃C₂T_x nanosheets treated with sodium L-ascorbate was orders of magnitude higher as compared to untreated ones after 21 days. Our findings have the potential to be generalized to protect other types of MXenes (in both the 312 and 211 families) as well and solve the most pressing challenge in the field of MXene engineering.

Key-2: Keynote Session-2

Time: Wednesday, 18/Aug/2021: 10:20am - 12:00pm · Virtual location: Theatre

Session Chair: Yu Huang

10:20am - 11:00am

Interfacial structure, interparticle forces and assembly dynamics during growth of hierarchical nanomaterials via oriented attachment

J. J. De Yoreo, L. Liu, G. Zhu, S. S. Kerisit, M.L. Sushko, J. Chun, E. Nakouzi, G.K. Schenter, J. Loring, B.A. Legg, K.M. Rosso, C.J. Mundy

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Assembly of inorganic nanocrystals to form hierarchical structures is a common approach to creating functional materials. This process exhibits diverse styles ranging from oriented attachment (OA) of like phases to mis-oriented aggregation of disparate phases followed by coarsening to ordered structures. While descriptions of these systems must share a commonality with continuum-based DLVO-type theories for simple colloids, nanocrystals present additional complexities, including face-specificity of dielectric properties, inherent dipolar interactions, structured nanoscale interfaces, and solvent-responses at a length scale comparable to particle size. To understand the relationship between interfacial structure, interparticle forces and assembly dynamics, we are investigating colloidal assembly of titanium-, iron- and zinc-oxides. AFM-based fast force mapping shows that solution structure exhibits sub-nm heterogeneities both along and perpendicular to crystal surfaces, reflecting gradients in speciation and water density that mediate interparticle forces. In situ TEM observations demonstrate that direction-specific forces attract and align diffusing ZnO nanoparticles at distances far in excess of what is expected based on DLVO theory. Particles start their approach from beyond 10 nm and undergo OA unopposed by any significant energy barrier. MD simulations on numerous systems predict that solvation forces are responsible for driving coalignment by creating orientation dependent solvent-separated minima. However, no attractive interactions are predicted beyond ~1 nm and the minima are separated by barriers of 100 kT or more, making it unclear why particles are attracted from long range and how contact is ultimately achieved. Classical density functional theory predicts that ion correlation effects decrease the barriers, enabling attachment, but do not predict long range attractive forces nor a preference for coalignment. We find that, in ZnO, the long range of the forces and torques and high degree of coalignment are both a consequence of an inherent dipole moment. Dipole-dipole interactions enforce alignment even in the absence of solvation-defined forces and drive attraction at large separations. Similar studies on iron-oxide/sodium-oxalate and gold/sodium-citrate show that addition of the organic ligands produces a dramatically different assembly pathway and outcome. The first particles to appear, either through seeding or nucleation from a precursor phase, become covered with the organic ligand, which creates interfacial gradients that drive all new particles to nucleate about 1 nm away from existing ones, to which they attach without a barrier. Consequently, aggregates of coaligned particles are formed with a shape reflecting differences in nucleation rate along distinct crystallographic directions.

11:00am - 11:40am Warning: The presentations finish prior to the end of the session!

MXenes – A Decade of Discovery and Expansion of 2D Materials

Yury Gogotsi

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A decade after the first report, the family of two-dimensional (2D) carbides, nitrides and carbonitrides (MXenes) includes structures with 3, 5, 7, or 9 layers of atoms in a variety of ordered or solid solution forms, including high-entropy systems. Dozens of MXene compositions have been produced, resulting in MXenes with mixed or uniform surface terminations. MXenes have shown useful and tunable electronic, optical, mechanical, and electrochemical properties, leading to applications ranging from optoelectronics, electromagnetic interference shielding, and wireless communication to energy storage, catalysis, sensing, and medicine. This lecture will present a brief overview of relations between structure, composition, properties and applications of MXenes. The challenges to be addressed will be discussed and research directions that will deepen the fundamental understanding of MXenes' properties and enable their hybridization with other 2D materials in various emerging technologies will be outlined.

**FESC-2: Functional Materials for Energy Storage and Conversion Devices**

Time: Wednesday, 18/Aug/2021: 10:20am - 12:00pm · Virtual location: AU 2410

Session Chair: Haimei Zheng

10:20am - 10:30am**A study on the meniscus stability of meniscus solution shearing coating for maximizing the crystal size of perovskite at high speed****Dong Soo Kim, I Ji Kim, Hyunah Lee, Min hun Jung**Hanbat National University, Korea, Republic of (South Korea); kds671@hanbat.ac.kr

Perovskite solar cells are one of the new and renewable energies. Many studies are underway because they have the advantage of being inexpensive in process cost by using inexpensive materials and enabling low-temperature solution processes. To mass-produce large-area perovskite solar cells, a high-speed process must be applied. However, in the case of perovskite materials, when fabricated in a high-speed process, the size of the crystals, which greatly affects the efficiency, tends to decrease, making it difficult to apply mass production [n(Roll to Roll process)]¹.

In this paper, a process study was conducted using the meniscus solution shearing process technology to fabricate a perovskite thin film having a large sized crystal even at high speed. The equipment used is an equipment using a meniscus formed by a capillary phenomenon of a gap between a substrate and a blade, and the stability of the shape of the meniscus is one of the factors that have many influences on the thin film². To confirm this, after setting the gap and the blade angle to various values among the process parameters of the equipment, the meniscus shape and the perovskite crystal change accordingly were confirmed. As a result of the experiment, a stable meniscus was confirmed at a blade angle of 3° and a gap of 100μm, and crystals having a crystal size of 10246.54μm² were obtained. However, at a blade angle of 10° and a gap of 500μm, the meniscus shape became unstable, and it was confirmed that the size of the crystal at this time decreases compared to that of the stable meniscus. Through this study, the optimum process conditions were established to produce a thin film of perovskite with large sized crystals even under a high-speed process of 20 mm/s. Compared with the low speed (~5mm/s) conducted in the previous study, a similar sized crystal was obtained to confirm the possibility of a high-speed process, which has great originality from the previous study

10:30am - 10:40am**Meta-material made super-capacitor that harvests nuclear particles kinetic energy and delivers it as electricity****Liviu Popa-Simil**LAAS, United States of America; laaos@laaos.org

Energy released in nuclear reactions is by one million times larger than that delivered in chemical processes, and using engineered nano-hetero structures it become possible to produce battery like systems. There are three types of batteries that can be produced, generically called:

- isotopic batteries, known for using nuclear transmutation reactions that release alpha or beta radiation, that is harvested and converted into electricity, previously known as alpha or beta voltaic, one such battery delivering the energy of more than 100,000 same power chemical batteries.
- fission batteries, delivering energy at demand, being in fact a solid-state compact nuclear reactor, where the meta-material inside is harvesting the energy of the fission products, which are over 200 times more energetic than decay reactions, and
- fusion batteries, where the meta-material is harvesting the energy of the fusion reactors, where fusion is up to three times more energetic than fission.

Complementary these meta-materials may be morphed on surfaces, able to convert particle beam energy, useful in space beamed power applications, and being hyperbolic meta-structures for some combinations they exhibit intense EM properties, being possible of emitting THz up to optical radiation.

There are many functional configurations of meta-materials that may be used, to convert moving particle energy into electricity as:

- planar structures, made of parallel nano-layers of materials, where for harvesting the energy of a 3 micron thick alpha emitter, as ²¹⁰Po, ²³⁹Pu, ²⁴¹Am, it takes a harvesting double foil of about 50 mm thick, useful for self-powered electronic modules, or long term batteries. For example using 40 g of pore ²³⁸Pu, it may produce a 200 g, 40cc, 15 W battery, able to power an artificial heart for more than 40 y, or 400 y lifetime batteries for space applications by using ²⁴¹Am. In a modified configuration, the meta-material may work similar to a laser emitting THz or visible radiation for the same lifetime for data communication purposes.
- nano-beaded structures, made of a distribution of nano-beads embedded into an amorphous dielectric structure, that have higher operating temperatures and efficiencies than planar structures, and
- heterogeneous nano-tube structures, believed to exhibit higher conversion efficiencies, over 90%, for isotropic radiation, but exhibiting real constructive difficulties, being now only a theoretical endeavor.

The project is in TRL=3 stage, having some simulations and ion beam tests accomplished, and more work is needed to develop the highly functional and reliable power sources.

10:40am - 10:50am**Bandgap engineering of amorphous sputtered hydrogenated silicon carbide thin films for photoelectrochemical water splitting**



Maria Del Carmen Mejia¹, Mario Kurniawman², Alvaro Tejada^{1,3}, Rolf Grieseler¹, Isabel Diaz⁴, Magaly Camargo⁴, Francisco Rumiche⁵, Andreas Bund², Jorge Andres Guerra Torres¹

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Bandgap engineering of undoped and Al doped sputtered amorphous hydrogenated silicon carbide (a-SiC:H) thin films was carried out to assess light absorption properties of the material by maintaining the silicon to carbon stoichiometry without compromising its photoelectrochemical water splitting capabilities. Properties tailoring was achieved by varying the hydrogen concentration in the semiconductor during the deposition process and through post-deposition thermal treatments. Optical constants were retrieved by suitable methods for the accurate determination of the fundamental absorption of dielectric thin films. Bandgap values were obtained by fitting the fundamental absorption using three different models, namely iso-absorption, Tauc and Band-fluctuations. Variations in the structure and hydrogen composition were tracked by Infrared and Raman spectroscopy techniques. Differences among bandgap values extracted by the distinct methods and their correlation to a-SiC:H structural features demonstrated that a structural disorder, rather than a hydrogen rearrangement or depletion, would be responsible for the observed annealing induced optical bandgap enhancement. The tuning of the optical bandgap of the p-doped a-SiC:H sample, with low hydrogen concentration, showed a gradual increase of the bandgap from 2.59 to 2.76 eV. The latter increase was induced upon the annealing steps from 200 °C till 600 °C. After heating at 600 °C the electric performance was strongly improved and required ohmic contacts were obtained. These bandgap values are close to the reported minimum bandgap necessary for water splitting taking into account overpotentials. We believe that these results will contribute to the design of monolithic tandem solar cells for water splitting applications.

10:50am - 11:00am

Peculiar Defects Behavior in Charge Recombination of Metal Halide Perovskites and Conventional Semiconductors

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Metal halide perovskites have attracted great attention due to their high and rapidly rising power efficiencies, as well as many other important advantages. Since the low-cost solution-based synthesis of the perovskites invariably introduces defects, a strong defect tolerance should exist in these materials. However, it is usually believed that those defects would form Shockley-Read-Hall (SRH) electron-hole recombination centers that decrease solar conversion efficiency. Herein we investigate the non-radiative recombination processes in both MAPbI₃ and CsPbI₃ using ab initio non-adiabatic molecular dynamics within real-time time-dependent Kohn-Sham formalism and surface-hopping framework. Regardless of whether the defects introduce a shallow or deep state in the band structure, we find that the charge recombinations in these perovskites are not enhanced which contrary to predictions of the SRH theory. We show that the strong tolerance of electron-hole recombination against defects is explained due to the combination of having low-frequency lattice phonons and weakly overlapping electron and hole states. Both factors significantly decrease the non-adiabatic coupling and inelastic electron-phonon interactions. The previous SRH models that work for the conventional semiconductors, fails for the metal halide perovskites because they do not explicitly include the electron-phonon coupling. Thus, we propose that other "soft" semiconductors, in particular, a small bulk modulus should exhibit defects properties similar to those of the perovskites.

11:00am - 11:10am

Harvesting electrical energy of carbon nanotube yarn in sea water for self-powered devices

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Mechanical energy harvesters are needed for such diverse applications as self-powered wireless sensors, structural and human health monitoring systems, and cheaply harvesting energy from ocean waves. We report carbon nanotube yarn harvesters that electrochemically convert tensile or torsional mechanical energy into electrical energy. The carbon nanotube yarn is lightweight, mechanically-robust and non-corrosive to be suitable for long time use in electrolytes including sea water. Fundamentally, these yarns are supercapacitors. In a normal capacitor, you use energy – like from a battery – to add charges to the capacitor. But in our case, when you insert the carbon nanotube yarn into an electrolyte bath, the yarns are charged by the electrolyte itself. No external battery is needed. When a harvester yarn is twisted or stretched, the volume of the carbon nanotube yarn decreases, bringing the electric charges on the yarn closer together and increasing their energy. This increases the voltage associated with the charge stored in the yarn, enabling the harvesting of electricity. Stretching the yarns 30 times a second generated 250 watts per kilogram of peak electrical power, when normalized to the harvester's weight. Our self-powered emergency signal device is based on the carbon nanotube yarn and technology as mentioned above. The product consists of a balloon part that floats the human body by buoyancy in the sea and a harvesting part that is connected with it and generates electricity by the swirling of sea water. The special thing about our products is in the harvesting parts. The carbon nanotube yarns harvest the mechanical energy of the ocean to produce electricity, store and boost electrical energy in the connected circuitry to drive electronic equipment like LED. Generated electricity could drive LED and air balloon like life jacket and it can increase the probability of survival in ocean emergency. The device harvests the mechanical energy from the movement of sea water and use it as electrical energy, so it has the advantage of being semi-permanent and safer. It can be used in all types of existing life-saving equipment such as marine leisure sports including surfing, navy, passenger ships and airplanes.

11:10am - 11:20am

Synthesis of anatase-rutile mixed phase TiO₂ photo-anode for dye-sensitized solar cells

Mian-En Yeoh¹, Kah-Yoong Chan¹, Venkatraman Madurai Ramakrishnan², Muthukumarasamy Natarajan², Hanabe Chowdappa Ananda Murthy³, Ruthramurthy Balachandran⁴

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As a promising alternative to the conventional silicon-based solar cells, dye-sensitized solar cell (DSSC) has attracted intensive research interests over the past decades owing to its facile and low cost fabrication process compared to the silicon chip manufacture. Generally, a DSSC consists of transparent conducting oxide (TCO) substrate deposited with titanium dioxide (TiO₂) film as photo-anode. Although the TiO₂ photo-anode can be conveniently prepared by using the commercial TiO₂ paste, there are several disadvantages about the commercial paste such as high cost and incapable of altering the TiO₂ composition through doping for enhanced photovoltaic performance. Hydrothermal method is the most widely adopted technique for the synthesis of TiO₂ photo-anode. Nevertheless, the reported processing steps for the hydrothermal synthesis of TiO₂ photo-anode were intricate and thus complicated the overall DSSC processing. In this work, we have developed a reinvented methodology for the synthesis of anatase-rutile mixed phase TiO₂ photo-anode by omitting several intermediate steps, which can simplify the whole DSSC processing significantly. By using the reinvented methodology, the DSSCs with promising photovoltaic performance were fabricated, which was comparable to the DSSCs based on commercial TiO₂ paste. In addition, it was discovered that the rutile content in the TiO₂ photo-anodes showed an increasing trend with prolonged hydrothermal durations. The improvement in DSSC efficiency with higher rutile content can be attributed to the synergistic effect between anatase and rutile phases in the DSSCs, in which the electron-hole recombination was inhibited by the electron transfer from rutile to anatase lattice trapping sites, thereby improving the photo-catalytic activity. This study offers a promising route to simplify the DSSC processing, as well as elucidating the influence of hydrothermal duration on the synthesis of TiO₂ photo-anode.

11:20am - 11:30am

Synthesis and Characterization of Polyacrylonitrile (PAN) Nanocomposite for Proton Exchange Membrane Materials in Fuel Cells

Seda Köksal Yeğin¹, Mualla Öner², Tomáš Remiš³, Martin Tomáš³, Tomáš Kovářik³

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Fuel cells (FCs) is the future potential promising candidate for a power source providing a renewable and clean energy for remote power supplies, portable power devices, stationary power generations, and a wide range of transportation applications (1). The membrane is one of the essential components in proton exchange membrane (PEM) fuel cells (2). Membranes should be high thermal stability, high protonic conductivity, low electronic conductivity, good mechanical properties to ensure the achievement of the fuel cell (3). Therefore reliability, stability and durability of the membranes used for PEM fuel cells are still under continuous assessments.

In this study, phosphoric acid doped polyacrylonitrile (PAN) nanocomposite membranes were prepared by dispersion of various amounts of fumed silica particles and borax decahydrate in PAN polymer matrix followed by phosphoric acid doping as the proton conducting agent. Electrochemical Impedance Spectroscopy (EIS), TGA, XRD, FTIR and SEM were used to characterize membrane samples produced by using electrospinning technique and solvent casting method. The results showed that the membranes have high performance relative to commercially available Nafion membrane.

References

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11:30am - 11:40am

Synthesis and Characterisation of Few Layer Pristine and Nitrogen Doped CVD Graphene for Supercapacitor Application

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Graphene has been explored extensively due to its astonishing electrical, optical, mechanical and thermal properties. Recently, it gained significant attention in the area of energy storage devices due to its high surface area, low cost and minimal environmental impact. In the current study, we have synthesized few layers pristine and nitrogen doped graphene on copper foils through Low Pressure Chemical Vapor Deposition (LPCVD) assisted approach for supercapacitor application. The FLG samples were transferred through PMMA (Poly(methyl methacrylate)) assisted copper etching method on the desired substrates for further characterisations. The nitrogen presence was confirmed through the SEM-EDS mapping and XPS data revealed the formation of graphitic-N, pyrrolic-N and pyridinic-N bonds.

The supercapacitor device was fabricated by sandwiching the PVA (Poly Vinyl Alcohol) hydrogel Na₂SO₄ electrolyte membrane between the two FLG samples on copper substrates as electrodes. The cyclic voltammetry and charge discharge characterisations



were performed for the estimation of specific capacitance and energy density and power density of the device. Cyclic voltammetry of the symmetric supercapacitor device fabricated by N doped CVD graphene exhibit high areal capacitance in the range of 0.9mF/cm² to 0.1mF/cm² at the scan rates ranging from 10 to 500 mV/s respectively.

Nitrogen doping in graphene resulted in the higher areal capacitance due to the enhancement in electrochemical activity in comparison to pristine graphene.

11:40am - 11:50am

Integration of electrostrictive bilayer composites into cantilever systems for mechanical energy harvesting

Annie Colin, Philippe Poulin, Mickael Pruvost

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Different transducers (electromagnetic, piezoelectric or electrostatic systems) are studied for decades to convert vibrational energy into electricity. But they suffer from several limitations, including difficult integration, brittleness, low efficiency or large electric losses. New energy harvesters are emerging, exploiting triboelectricity [1] or electrostriction [2]. As triboelectric systems are very sensitive to humidity [3] and present large impedances [4], studying other transducers as electrostrictive systems makes sense. Indeed, the flexible and stretchable nature of electrostrictive polymers makes them good candidates for developing highly sensitive generators, with greater integration ease. We design a new material by preparing a PDMS porous material of closed porosity by using an emulsion road [5,6]. The surface of the closed pores is covered by carbon black conductive particles. We use the material as a dielectric layer in a capacitance whose value varies due to the vibration of a cantilever. This induces back and forth displacement of electrons and thus production of energy along a cycle. We are demonstrating that this structure provides a positive energy balance thanks to a non-conventional bilayer structuration of the active material. We measured a net power of 2.8 for an acceleration of 3 g and a frequency of 25 Hz under a low bias voltage of 64 mV/. The low resonant frequency of the triangular cantilever, makes the device promising for ambient energy harvesting. In addition, the low-cost process and low toxicity are criteria encouraging their future development.

11:50am - 12:00pm Warning: This presentation lies outside the session time!

Computational Modeling of Two-Dimensional Materials for Sustainable Energy Storage

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Two-dimensional materials (2DM) such as graphene, transition metal dichalcogenides (TMD), MXenes, and their heterostructures are among the most promising energy materials for the radically advanced batteries. In this talk, two important computational aspects of 2DM-based batteries are addressed – (i) 2DM as anode materials, and (ii) 2DM as van der Waals (vdW) slippery interface. The conventional anode materials have several problems, such as low gravimetric capacity (e.g., graphite – 372 mAh/g) and high volume expansion (e.g., silicon – 300%). Our computational modeling shows that topologically modified 2DM can be utilized as high-capacity anode materials for ion batteries with capacity as high as 1000 mAh/g. However, despite enormous opportunities in 2DM anode, several challenges need to be addressed, such as trapping of adatoms at the defect sites, the effect of defects on the diffusivity of adatoms, mechanical degradation at defect sites during charging/discharging, etc. The second part of the talk discusses the interface of anode and current-collector (e.g., silicon anode and copper current-collector in Li-ion battery). To combat the issue of high-stress development at the anode-current collector interface during charging/discharging, we propose the usage of the graphene layer over the current collector as a vdW slippery interface that reduces the interfacial stress and enhances the cycle life of batteries. Our computational results are in excellent agreement with the experimental findings.

FLNM-INV-1: Fabrication of Low dimensional, Nano and 2D materials

Time: Wednesday, 18/Aug/2021: 10:20am - 12:30pm · Virtual location: AU 2412

Session Chair: Albert Wang

10:20am - 10:35am

Semiconductor to Topological Insulator Transition in Transition Metal Dichalcogenides Core-Shell Lateral Heterostructures

Xi Dong, Wei Lai, Pengpeng Zhang

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Polymorphic phase transition is an important route for engineering the properties of two-dimensional materials. Heterostructure construction, on the other hand, not only allows the integration of different functionalities for device applications, but also enables the exploration of new physics arising from proximity coupling. Yet, implementing a design that incorporates the advantages of both remains underexplored. In light of integrating heterostructure formation and phase engineering in one step, we demonstrate a novel phase transition technique based on the construction of lateral (WSe₂/SnSe₂) core-shell architecture by molecular beam epitaxy. A semiconductor to topological insulator (TI) transition associated with the polymorphic change of WSe₂ core is revealed by scanning tunneling microscopy/spectroscopy in conjunction with first-principles calculations. Since the proposed phase transition mechanism only fundamentally requires a van der Waals interacting substrate and sufficient core-shell lattice mismatch, the approach could be potentially versatile towards other transition metal dichalcogenides and vapor deposition methods.

Key Words: Phase engineering, TMDs, Topological Insulator

Reference:

1. Dong, X.; Lai, W.; Zhang, P. P., Semiconductor to Topological Insulator Transition Induced by Stress Propagation in Metal Dichalcogenide Core-Shell Lateral Heterostructures. Materials Horizons DOI: 10.1039/D0MH01688H (2021).

10:35am - 10:50am

Ultrafast Mid-infrared Fibre Lasers Based on 2D Nanomaterials

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We report on the development of wavelength-stabilized all-fibre ultrafast mid-infrared laser systems that utilize MXenes and platinum diselenide (PtSe₂) as novel two-dimensional saturable absorber materials for passive mode-locking.

The linear laser cavity consists of a high reflective femtosecond laser inscribed chirped fibre Bragg grating that provides wavelength selective feedback which is essential for stable operation. The observed mode-locked pulse train from this erbium-doped fluoride fibre laser cavity has a 30 MHz repetition rate with an average power of 603 mW and a transform-limited pulse duration of around 10 ps. Our results highlight the feasibility of using novel two-dimensional nanomaterials such as MXene and PtSe₂ as promising candidates for the realization of all-integrated ultrafast fibre laser systems for the technically important mid-infrared wavelength region.

10:50am - 11:05am

Molybdenum Disulfide Nanoribbons: Fabrication, Manipulation, Assembly and Beyond

Donglei (Emma) Fan

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In the past decade, molybdenum disulfide (MoS₂) has received intensive attention owing to its unique physical and chemical properties that enable applications ranging from optoelectronics to catalysis, energy storage, and environmental remediation. Being capable of manipulating MoS₂ nanostructures and assembling them at designated locations as building blocks for advanced devices is essential for realizing their applications. Herein, we report an innovative and robust approach to synthesize large-scale MoS₂ nanoribbons with tunable dimensions. The strong shape anisotropy of the long-shaped MoS₂ allows intense electric polarization that endows them with facile manipulation with the electric tweezers based on combined AC and DC fields. The nanoribbons transport following prescribed patterns with precision positioning and angular control; they rotate both clockwise and counter-clockwise at different AC frequencies. Such a versatile manipulation of MoS₂ (or any 2D materials) has been reported for the first time. Furthermore, the mechanical electrorotation behaviors of the MoS₂ strongly correlate to their electronic type that supports their semiconductor nature. This is further confirmed by their rapid optoelectronic response to light from 450 nm to 750 nm. In parallel, owing to the polycrystalline nature of the MoS₂ nanoribbons that carry abundant surface defects, they can be readily functionalized and assembled between microelectrodes with UV-light-triggered click-chemistry and remove Mercury from water efficiently. Overall, this research unveiled an innovative synthesis, manipulation, and assembly scheme of MoS₂ that could be applied to various 2D transition metal dichalcogenides (TMD).

11:05am - 11:20am

Semimetals for Nanoelectronics Applications

Farzan Gity, Lida Ansari

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The electronics industry has relied for over fifty years on shrinking transistor geometries for improvements in circuit performance while reducing cost per function. The conventional idea of using a fixed material set and scaling devices in length as expressed by Moore's

"law" [1] to reduce costs while enhancing the performance came to an end effectively during the mid-1990s for the manufacture of integrated circuits relying on field-effect transistors (FETs). As miniaturization continues to ultra-scaled transistors, the concept of doping to form junctions fails and forming heterojunctions becomes extremely difficult. In semimetals on the other hand, quantum confinement induced bandgap leads to a semimetal-to-semiconductor transition which can be utilized as a novel means for making dopant-free monomaterial rectifying junctions and forming a FET near atomic dimensions. These properties open up new opportunities in bandgap engineering for future nanoelectronic devices.

For atomic-scale device lengths, applying classical continuum models, e.g., the Ohm's law, will no longer be valid and quantum mechanics must be applied to describe the electron transport correctly. This makes nanoscale components conceptually different from larger devices as device dimensions approach the Fermi wavelength of the electrons. Schottky barrier at the interface of bulk-like 'source and drain' regions, and quantum confined 'channel' region in a monomaterial film allows for forming Schottky barrier transistors with critical dimensions of a few nanometer using techniques consistent with advanced nanoelectronics manufacturing.

Our recent studies on semimetal nanostructures, demonstrate that ultra-thin Bi films and semimetallic transition metal dichalcogenides (TMDs) such as PtSe₂ and PtTe₂ have distinct thickness-dependent electronic structures and physical properties [2-5]. Although the bulk crystal is a semimetal with an overlap of the conduction and valence bands, monolayer PtSe₂ and PtTe₂ have been revealed to be a semiconductor. The possibility of making semimetal hetero-dimensional junctions with uniform chemical bonding at the interface promises the possibility of fabricating ideal Schottky barriers [6,7].

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11:20am - 11:35am

Nanosized semiconductors as functional materials for gas sensing

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The great expectations of the gas-sensor market have fostered research in material science and technology toward constant development. In particular, the search for materials should accomplish high sensitivity and low-power consumption. In the last years, a wide plethora of sensing materials has been developed, from traditional (e.g. ceramic thin/thick films) to nanostructured (e.g. nanowires, nanosheets, nanoflowers) semiconductors, including novel low-dimensional semiconductors (e.g. graphene, black phosphorus, metal organic frameworks).

The great challenge of low-dimensional nanostructured materials lies in the control of their properties by the morphology and the grain size, which combines bulk and surface effects. One-dimensional nanostructures are ideal for investigating the dependence of electrical transport, mechanical and optical properties on size and dimensionality. Two-dimensional nanostructures are ideal components for nanoscale devices, due to their high surface-to-volume ratio, fascinating photocatalytic and optical activities.

Most common conventional gas sensors are based on three-dimensional Metal Oxides (MOX). These devices are low-cost and provide high sensitivity, but they suffer of poor stability over the time and need high power consumption to heat up the transducer for recovery, which restricts their use in portable sensing systems. The performance of MOX-based sensors depends crucially on their dimensions, morphology, composition, and surface activity. Among the several parameters that influence the sensing properties of a MOX sensor, the potential barrier at the interface between grains is a major physical quantity. In this sense, the broad assortment of one-, two- and three-dimensional MOX nanostructures has been a precious source for gas sensors technology, which owes its constant development to the requirements of physical, chemical and biological detection systems.

11:35am - 11:50am

On-surface synthesis of small bandgap graphene nanoribbons

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Graphene nanoribbons (GNRs), quasi-one-dimensional strips of graphene with atomically precise width, exhibit unique electronic and magnetic properties depending on the edge structure and width of the GNRs. Armchair-edged GNRs (AGNRs) with finite bandgaps have attracted much attention for their potential reliability as organic semiconducting materials. After the first report of bottom-up synthesis of anthracene GNR (7-AGNR, where 7 is the width measured by the number of rows of carbon atoms across the AGNR) by on-surface-assisted polymerization and subsequent cyclodehydrogenation of precursor monomers on metal surfaces in 2010, many attempts have been reported to control the bandgap of AGNRs by the edge modification, control of the ribbon width, and the insertion of heteroatoms to AGNRs.

From theoretical calculation, the wider AGNR was predicted to have smaller bandgap size. We started with the synthesis of bis-diketone precursor of 7,16-dibromo-heptacene for the on-surface synthesis of 15-AGNR, but heating of the precursor on Au(111) surface offered hepta-cene organometallic complex instead of 15-AGNR.² The steric hindrance between precursors prevented the polymerization of the precursors and gold atoms were inserted between the monomers. In 2020, we were successful in the first on-



surface synthesis of 17-AGNR using 1,2-bis-(2-anthracenyl)-3,6-dibromobenzene as a monomer and in characterization of 17-AGNR by combining in situ scanning tunneling microscopy and spectroscopy (STM/STS) and ex situ non-contact atomic force microscopy (nc-AFM).³ We revealed that the 17-AGNRs have a bandgap of 0.19 eV on Au(111), which is consistent with a theoretically obtained bandgap of 0.63 eV for a freestanding 17-AGNR.

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11:50am - 12:05pm

PdSe₂: a Pentagonal Layered Material Bridging the Gap Between 2D and 3D Materials

Liangbo Liang, Kai Xiao, Alexander Puzetzy, An-Ping Li, David Geohegan, Bobby Sumpter

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PdSe₂ is a new layered material with an in-plane pentagonal network and stronger-than-vdW interlayer coupling. It offers great trade-off between carrier mobility, band gap, and air stability for nanoelectronics [1]. Because of its unique atomic structure and strong interlayer coupling, it behaves like 2.5D material and many of its properties are different from those of commonly known 2D materials, such as graphene and MoS₂. Here I will highlight how first-principles modeling/simulation guided experiments to explore its structural, electronic, and vibrational properties. Because of strong interlayer coupling, its electronic band gap varies significantly from 1.3 eV (monolayer) to 0.06 eV (bulk), based on calculations and measurements [1]. For 2D graphene and MoS₂ that have weak interlayer interactions, the layers are quasi-rigid in low-frequency interlayer vibrations, which can be described by a linear chain model (LCM); however, in PdSe₂ the layers are no longer quasi-rigid, according to our Raman scattering calculations and measurements. Therefore, the thickness dependence of the interlayer Raman modes' frequencies in PdSe₂ deviates significantly from the LCM. A revised LCM was developed to account for the layer non-rigidity [2]. Finally, our calculations found that the pentagonal structure and strong interlayer coupling lead to low diffusion energy barriers for defects, and hence both intralayer and interlayer hopping of defects can occur relatively easily in PdSe₂ compared to MoS₂, as observed by scanning tunneling microscope (STM) [3]. Interestingly, the high mobility of defects and strong interlayer coupling in PdSe₂ also contribute to phase transition to multiple different structures: including 2D PdSe₂, 3D PdSe₂, and 1D pentagonal PdSe₂ nanoribbons, as corroborated by our DFT calculations and the atomic-scale STM simulations [4]. Our joint theoretical/experimental works demonstrate that PdSe₂ is a novel layered material featuring great transistor performance, strong interlayer coupling, versatile phase transition, etc.

12:05pm - 12:20pm **Warning: The presentations finish prior to the end of the session!**

Ultrafast control in THz graphene-based metasurfaces

Anna TASOLAMPROU¹, Anastasios Koulouklidis¹, Eudokia Kyriakou^{1,2}, Christina Daskalaki¹, M. Said Ergoktas^{3,4}, Coskun Kocabas^{3,4,5}, Maria Kafesaki^{1,2}, Stelios Tzortzakis^{1,2,6}

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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 various 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. Here we present that ultrafast modulation response in a graphene thin film absorber which can be assessed with use of a broadband THz time-domain-spectroscopic system (THz-TDS) in an IR pump-THz probe configuration. The simple structure consisting of a graphene sheet is placed over a back plated dielectric substrate, forming an electromagnetic cavity. The cavity provides the means for achieving critical coupling and hence increased 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. For example it has been shown, that using the IR pump-THz probe configuration in hybrid metasurfaces with metals combined with photo-conducting semiconductors one is able to produce switchable and tunable terahertz electromagnetic functions.

EPMM-1: Electronic, Photonic and Magnetic Materials

Time: Wednesday, 18/Aug/2021: 1:00pm - 3:00pm · Virtual location: AU 2410

Session Chair: Wanli Yang

1:00pm - 1:10pm

Magnetocaloric Effect, Magnetothermal and Elastic Properties of SmFe₃ and ErFe₃ Compounds

Mohammed Said Mohammed Abu-Elmagd¹, Fatema Z. Mohammad², A. Abdel-Kader Ahmed³, Tarek Hammad³, Sherif Yehia³, Samy H. Aly²

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We report, using the mean field theory, on the magnetothermal properties of the ferromagnetic SmFe₃ ($T_c \approx 600$ K) and ferrimagnetic ErFe₃ ($T_c \approx 600$ K, compensation temperature ≈ 230 K) compounds, e.g. the temperature and field dependence of magnetization, magnetic specific heat and magnetic entropy. The Magnetocaloric effect (MCE) i.e. the isothermal change in entropy (ΔS_m) and the adiabatic change in temperature (ΔT_{ad}) are then calculated using the trapezoidal method and standard relations involving the total specific heat of these systems. The electronic and lattice parts of the total specific heat and total entropy are calculated using the, ab-initio calculated, electronic coefficient of the specific heat γ_e and the Debye temperature Θ_D . The elastic constants, bulk and shear moduli are also ab-initio calculated using the Density Functional Theory, as implemented in the Wien2k code. Both direct and inverse MCE effects are found in the ferrimagnetic ErFe₃, while only direct MCE effects are found in SmFe₃. Maximum ΔS_m , for a 60 kOe field change, is about 1.15 J/mol.K for SmFe₃. Maximum direct and inverse $|\Delta S_m|$ for ErFe₃ are around 0.4 J/mol.K for the same field change. The order of the magnetic phase transition in these two system will be discussed in the light of specific features of the thermomagnetic and magnetocaloric properties together with the Arrott plots and universal curves of both systems.

1:10pm - 1:20pm

Particle production and characterization for Transcatheter Arterial Chemoembolization applications: comparison of magnetic nanoparticles and clay mineral particles.

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In Transcatheter arterial chemoembolization (TACE) procedure, micron-sized (at least 20 μm) particles and chemotherapeutic agents are injected into arteries that supply oxygen and nutrients to the tumor site. Resulting ischemia and chemotherapy leads to tumor size reduction or necrosis. Arterial embolization is currently performed clinically for the treatment of some cancer types such as liver, kidney tumors yet the particles that are used are mostly polymer beads loaded with chemotherapeutic agents. Multifunctional particles and/or particles with improved drug loading and releasing properties that are also radiopaque, could significantly improve the outcome and increase the efficacy of TACE procedures. In our search for development of improved TACE particles, we used magnetic nanoparticles and clay micro-particles due to their unique properties. Firstly, magnetic micro-particles suitable for TACE applications were produced via bridge flocculation of nanoparticles and drug loading onto their biopolymer coated surfaces. Later clay mineral micro-particles were prepared by loading chemotherapeutic agents and X-ray contrast agents onto their surfaces while controlling their sizes to be applicable TACE applications. Two different structures that are produced were characterized conventionally and in vitro. Furthermore, both produced magnetic micro-particles and clay mineral micro-particles were tested in vivo (rabbit renal model) for embolization and drug delivery efficacy. Results indicated that both structures could achieve embolization, were traceable via X-ray or Magnetic Resonance imaging techniques, and could release drug at the target site. In addition, in vitro cell viability assays carried out for both particles showed no significant toxicity to healthy cells at low concentrations while drug loaded particles behaved like pure forms of the loaded drug against cancer cells. Both particle structures demonstrated specific properties. For example, while magnetic particles enabled magnetic hyperthermia and demonstrated slightly rapid drug release at the target site, clay minerals were biocompatible, possessed extremely high drug loading capacities and significantly extended drug release profiles. These specific properties should be considered before selection of the particles depending on the wanted outcome of TACE procedures.

1:20pm - 1:30pm

Novel Magnetisms in Mixed 3d-5d Transition-Metal Compounds

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Combining traditional and relativistic Mott insulators is presented here as a promising route to novel magnetic properties. Such materials could for example naturally take the form of the double-perovskite-like structure $AB_1-xB'_xO_3$ or the $ABO_3/AB'O_3$ heterostructure epitaxy films where $B=3d$ and $B'=5d$ transition-metal elements. The key mechanism is unusual exchange pathways opened by mixed spin-orbit coupling strengths on the 3d and 5d atoms, as demonstrated in our first-principles-based theoretical analyses of experimental data [1-3]. This renders a spin-flop transition from in-plane to out-of-plane alignment of magnetic moments in Sr_2IrO_4 upon substitution of Mn or Ru for Ir [1]. In Sr_3CuIrO_6 , the alternating placement of Cu and Ir ions turns isotropic antiferromagnetic superexchange between real spins to anisotropic ferromagnetic exchange between low-energy effective spins [2]. The spin-orbit-entangled isospins of the Ir ions have a negative g-factor of $g = -3$, opposite to the usual $g = 2$ on the Cu ions, making this spin-1/2 Ising-like ferromagnet surprisingly exhibit magnetic frustration in the uniform magnetic field and behave like a ferrimagnet with an antiferromagnetic Curie-Weiss temperature. This system also features an exotic magnetic-field driven critical point at which one half of the spins are frozen into a complete order and the other half are fully disordered at zero temperature. The response of this new state to transverse exchange perturbation provides a unique way to realize the long-sought pure XY model system [3].

Key Words: Mott insulator, spin-orbit coupling, opposite g-factors

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1:30pm - 1:40pm

Nonlinear optical properties of nanostructured titanium dioxide embedded Poly(methyl methacrylate) using the Z-scan technique

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The nonlinear optical properties of polymers are very important mainly due to their applications in photonic devices. Embedded nano particles in polymers extremely increase surface area because of proportionally more surface atoms than their microscale counterparts, thus allowing intimate interphase interactions and conferring extraordinary properties to the polymer. In this study thin film of Poly(methyl methacrylate)(PMMA) embedded with nanostructured titanium dioxide at various molar concentration was synthesized using casting method.

Nonlinear optical properties, such as nonlinear absorption coefficient, nonlinear reflective index and third-Order nonlinear optical susceptibility of these nanostructured titanium dioxide embedded Poly(methyl methacrylate) thin films using the Z-scan technique were measured. In this measurement CW green laser of 532 nm wavelength and 100 mW power was used in the Z-Scan. The results are useful for application of such polymer in optoelectronics devices.

1:40pm - 1:50pm

Access to Fluorescent Organic Push-Pull Chromophores with White Light Emitting Property Using Urea as the Electron Donor

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Molecular electronics is being actively pursued in order to miniaturize the electronic world. Organic molecular electronics is promising over inorganic due to unlimited possibility for bandgap tunability, cost effectiveness and easy processability. Conjugated organic push-pull chromophores consisting of Donor and Acceptor functionalities at the terminal positions have been tremendously explored from the past two decades because of their unique features in future generation materials, such as non-linear optical (NLO), Electro-optic piezo chromic materials and solar cells etc.¹ Luminescent, in particular white light emitting materials find significant attention owing to their applications in lighting and display.²

Last decade has witnessed a tremendous interest in donor substituted poly-cyano olefins based push-pull chromophores owing to its click type synthesis, high intramolecular charge-transfer (ICT), redox behavior and more importantly with high thermal stability.³ However, due to strong ICT, they generally does not exhibit luminescence. Unlike N,N-dialkylamino group, a bench mark organic donor alkyne,³ Our design strategy offers easy access to further functionalization on these chromophores and exhibits luminescence property apart from the inherent properties like ICT band and redox behavior.⁴ Herein, we present a new strategy that we adopted to obtain the same. The below figure shows the regardless of weak donor, the push-pull chromophores exhibited white light emission in solution without any complicated composites or conditions, as simple fluorescent organic molecules rarely exhibit such emission.

1:50pm - 2:00pm

Achieving Conformational Control in RTP and TADF Emitters by Functionalization of the Central Core

Nadzeva Kukhta^{1,2}, Rongjuan Huang², Andrei Batsanov², Martin Bryce², Fernando Dias²

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Nowadays, a manifold of fluorescent emitters has been developed for optoelectronic applications including organic light emitting diodes,¹ sensing,² probes for fluorescent imaging³ and optical thermometry.⁴ However, most of the emitters follow the singlet decay channel only, thus limiting the efficiency. Therefore, there is a need for alternative ways to harvest both singlet and triplet excited states. Thermally activated delayed fluorescence (TADF) is currently the leading strategy offering internal quantum efficiency (IQE) of 100% using purely organic emitters.⁵ In turn, efficient room temperature phosphorescence (RTP) can be realized when the molecular vibrations causing non-radiative T1→S0 relaxations are suppressed and efficient intersystem crossing (ISC) from S1 to T1 is promoted.⁶

The current work presents a new molecular design approach aimed at preventing the formation of multiple axial and equatorial conformers while employing the phenothiazine donor in a D-A-D system with the 9,9-dimethyl-thioxanthene acceptor unit. By introducing pertinent substituents onto the acceptor and altering the linking position of the donor moiety efficient RTP emitters with solely equatorial conformation were obtained. Moreover, functionalization of the thioxanthene with electron deficient groups resulted in a negligible ΔEST, enhanced reverse ISC (RISC) rate and efficient yellow TADF. A thorough photophysical investigation is provided. Theoretical calculations assist the understanding of the observed results.

Key Words: Fluorescence, Phosphorescence, Molecular Conformation

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2:00pm - 2:10pm

Long carbon fibers loaded ultra-porous epoxy composite for planar microwave absorber materials

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Recently, absorber materials are being used widely in several applications, for example, electromagnetic compatibility, stealth and anechoic chamber etc... However, absorption in a wide frequency range, especially low frequencies, is still a constraint for such applications, and materials with significant thickness are often necessary to guarantee an acceptable absorption. So, today, the challenge for these absorbers is to obtain the best compromise between three factors: thickness, mass and performance.

In our team, a new absorber material made from rigid epoxy foam filled with a very low concentration of carbon fibers (CFs) is developed in order to replace the flexible polyurethane foam currently available as commercial absorber. This solution has been proposed in order to compensate the flexibility of these commercial absorbers which limits the precise machining process, and therefore the use of complex geometries to improve absorption performance. Our results show a very good microwave absorption performance of our materials compared with the commercial one. However, the density of the proposed material remains one of the restraints that must be optimized.

In this work, a promising methodology to fabricate ultra-porous CF/epoxy foam composite with a very high EM absorbing performance is presented [1]. The results show that the pore size and the density of the composite can be controlled; here, the material density can be reduced by half compared to the standard density of used epoxy foam. Furthermore, samples with different CFs loads, with different lengths, are elaborated and characterized in free space in order to investigate the influence of CF length and cell structure on dielectric properties of composites [1, 2]. The reflection coefficient and dielectric properties were extracted and compared with those of the dense CF/epoxy foam. Moreover, the suitable properties that ensure an impedance gradient are selected to make a multilayer prototype composed of 5 layers. The simulation and measurement of this very lightly loaded multi-layer prototype were compared over the wide frequency band 2-16 GHz; results were compared to those of the dense CF/epoxy foam multilayer and also to those of commercial multilayer absorber.

2:10pm - 2:20pm

Long Time-Scale Magnetization Reorientation in Ferromagnetic Thin Films Induced by Chiral Molecules Adsorption

Nir Sukenik¹, Idan Meirzada², Galya Haim¹, Shira Yochelis¹, Oded Millo², Lech Tomasz Baczewski³, Nir Bar-Gill², Yossi Paltiel¹

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Chiral molecules act as spin filters and spin polarizers for electrons passing through them. This phenomenon is known as the chiral induced spin selectivity (CISS) effect.¹ Another aspect of the same effect, demonstrated magnetization reversal in a ferromagnet (FM) with perpendicular anisotropy after chemisorbing a chiral molecular monolayer without applying any current or external magnetic field.² This phenomenon was observed when the easy axis of the FM was out of plane, and immediately after the adsorption process. This raises two questions: what effect does the easy axis have on the adsorption and magnetization reorientation, and, more importantly, is this effect due to the bonding event, held by the FM, or a long timescale effect stabilized by exchange interactions. We performed vectorial magnetic field measurements of the magnetization reorientation of a ferromagnetic thin film exhibiting perpendicular anisotropy due to CISS using nitrogen-vacancy (NV) centers in diamond, following the time dynamics of this effect. In parallel, we have measured the molecular monolayer tilt angle in order to find a correlation between the time dependence of the magnetization re-orientation and the change of the tilt angle of the molecular monolayer.³ Furthermore, the effects of the ferromagnetic easy axis direction on both the monolayer tilt angle and the magnetization reorientation of the magnetic substrate, were studied using magnetic atomic force microscopy (MFM).⁴ Results show that changes in the magnetization direction correspond to changes of the molecular monolayer tilt angle, and a clear correlation between the ferromagnetic layer easy axis direction and the tilt angle of the bonded molecules, providing evidence for a long-timescale characteristic of the induced magnetization reorientation. These results show that exchange interactions that are generated by the CISS effect can stabilize surface spins over long periods of time. The strong interaction between chiral molecules and FMs in static systems can pave the way for using the CISS effect in the fields of memory devices and spintronics.

2:20pm - 2:30pm

Luminescence activation of terbium doped indium tin oxide and its impact on the host's optical and electrical properties

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The effect of terbium doping on the electrical, optical, and light emission properties of sputtered indium tin oxide thin films was investigated. The films were prepared by radio frequency dual magnetron sputtering maintaining a high optical transmittance in the ultraviolet and visible spectral regions and an electrical resistivity ranging from of 5×10^{-3} to $0.3 \Omega\text{-cm}$. Terbium-related luminescence is achieved after thermal treatments in air at 470°C at atmospheric pressure. Electrical resistivity and optical transmittance were registered after each annealing step to evaluate the compromise between the achieved light emission intensity, electrical and optical properties. Additionally, Tb-related luminescence thermal quenching is assessed by temperature-dependent photoluminescence measurements, from -190°C to 300°C , under non-resonant excitation. Thermal quenching activation energies suggest an effective energy transfer mechanism from the ITO host to the rare-earth ions. This indirect excitation mechanism is tentatively modeled using a spherical potential well, as well as a tight-binding one-band approximation, approach for a short-range charge trapping process and subsequent formation of bound excitons to rare-earth ions clusters.

2:30pm - 2:40pm

Optical and electrical properties analysis of sputtered tin-doped indium oxide thin films taking into account growth induced inhomogeneities

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Indium tin oxide (ITO) layers were prepared by radio frequency magnetron sputtering on fused silica substrates at low substrate temperatures in order to induce and assess the variation of the optoelectronic properties by post annealing treatments in an argon atmosphere. These layers show a growth induced inhomogeneous microstructure, which impacts the optoelectronic properties of the system [1]. The lowest resistivity measured by four-point probes obtained in this work was $2.5 \times 10^{-4} \Omega\text{-cm}$ after heating in argon at 500°C . Optical transmittance, elemental composition and electrical resistivity measurements were performed after each annealing step. In this work charge carrier density and carrier mobility were monitor after each annealing temperature by an optical analysis in which the films are treated as a two layers stack with different Drude parameters. Additionally, the intrinsic band-gap, Burstein Moss shift and valence effective mass are determined [2]. It was found that the optical band-gap energy increases with increasing carrier density for carrier densities above a critical value. Optical parameters such as refractive index, absorption coefficient, and band gap were estimated accordingly at each annealing temperature.

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2:40pm - 2:50pm Warning: The presentations finish prior to the end of the session!

Application of analytical modeling in probabilistic design for reliability of electronic and photonic materials, assemblies, packages and systems

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Merits, attributes and challenges associated with the application of analytical ("mathematical") predictive modeling in electronics and photonics materials science and engineering are addressed. It is shown that application of analytical modeling enables revealing and explaining the underlying physics associated with often non-obvious, always non-trivial and in some cases even paradoxical, problems. Some of the addressed problems are: interfacial thermal stresses in adhesively bonded or soldered assemblies and application of inhomogeneous attachments for lower thermal stresses [1,2]; thermal and lattice mismatch stresses in semiconductor crystal grown assemblies [3,4]; dynamic response of electronic systems to shocks and vibrations [5,6]; stress relief in solder joints owing to their elevated stand-off heights and inhomogeneous solder joint systems for lower thermal stresses [7,8]; stress relief in thermoelectric module designs [9,10]; low-temperature micro-bending of long-haul dual-coated optical fibers [11]; two-point bending of optical fiber specimens [12,13]. It is concluded that analytical modeling occupies a special place owing to its ability to provide clear and concise information of the problems it addresses. The general concepts are illustrated by practical numerical examples.

Key Words: Analytical Modeling, Electronic Materials, Photonic Materials, Physical Design for Reliability, Accelerated Testing

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FCM-1: Functional Composite Materials

Time: Wednesday, 18/Aug/2021: 1:00pm - 3:00pm · Virtual location: AU 2412

Session Chair: Donglei Fan

1:00pm - 1:10pm

1D and 2D Nanocarbon Alignment for Multifunctional Composites

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Nanoparticle alignment can benefit mechanical stress transfer, electron or photon transport, targeted drug delivery, enhanced Raman signals, among many other applications. Currently used methods such as electrical or magnetic fields are limited due to the requirement of responsiveness of nanoparticles, thus significantly limited the choices of materials that can be used in structural or functional composites. This talk will cover two novel manufacturing methods that can achieve preferential alignment of 1D and 2D carbon nanoparticles, respectively. The first example will be the use of 1D carbon nanofibers in the 3D printing technique. Our approach will be based on the use of stereolithography (SLA) in generating surface patterns and the utilization of layer-by-layer (LBL) assembly to selectively deposit the nanofibers on desirable locations. The drying thermodynamics and the confinement effects from the surface template arranged the nanoparticles with different morphologies and preferentially oriented nanofibers were observed with the control of inter-nanoparticle interactions. The second demonstration involves the alignment of 2D graphene that is challenging to obtain as compared with their allotropes, carbon nanotubes. Free-standing graphene will fold, crumple or wrinkle at ambient temperature due to their instability of thermodynamic states. Our manipulation of nanoparticle-polymer interfacial interactions will first constrain the graphene layers within specific region, followed by the macromolecular movements-generated shear and rotating moments, thus producing aligned graphene layers laminated between polymer channels. These two projects depend on our design and development of in-house manufacturing setups. The processed composite fibers and films were examined with their nanoparticle alignment, the mechanical reinforcement, and the functional properties (i.e., electrical conductivity, sensing of mechanical strains, chemicals, and VOCs). The unique manufacturing and composites have broad applications in wearable, robotics, biomedical, and other areas.

Key Words: Carbon, fiber, 3D printing, sensor

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1:10pm - 1:20pm

Composite laminate materials with low dielectric loss: theoretical model and dielectric characterization

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Organic matrix composite materials have a dominant position in the transport sector. These materials, mainly made of reinforcement fibers impregnated by a thermosetting resin, allow the fabrication of lightweight and mechanically resistant structural panels. Moreover they promote embedded electronic applications. With a societal and technological evolution ever more connected, the integration of antennas within load-bearing composite panels is a major area of interest. A few works have developed this original approach. Manac'h and al. [1] demonstrated similar microwave performance between a pure composite laminate antenna and a copper antenna in the 600 MHz – 2.1 GHz frequency band. Other antennas have been made from sandwich composite panels directly embedded within vehicle structures [2]. The present work aims to theoretically and experimentally study various dielectric composite laminate panels that may be used as support (substrate) and/or radome of antennas operating at microwaves. Composite laminate materials have been manufactured with E-glass, S2-glass and quartz fibers, impregnated with polyester, epoxy and urethane acrylate type resins by the standard vacuum infusion process. The two-dimensional Maxwell-Garnett's law [3] has been developed to theoretically retrieve the dielectric characteristics (permittivity ϵ_r and loss tangent $\tan \delta$) of the above composite laminate materials at 1 GHz. The experimental study of the composite materials has then been carried out over two frequency bands through impedance measurement (100 MHz – 1 GHz) and free space method (18 GHz – 26 GHz). Dielectric permittivities ranging from 3.0 to 4.3, and loss tangents from 3×10^{-3} to 1.3×10^{-2} have been measured. Experimental results are compared with those retrieved from the theoretical model. A strong fit on ϵ_r and $\tan \delta$ values is achieved, demonstrating the relevance of the 2D Maxwell-Garnett model. Moreover a permittivity $\epsilon_r = 3.1$ and a loss tangent $\tan \delta = 3 \times 10^{-3}$ at 1 GHz, and ($\epsilon_r = 3.2$; $\tan \delta = 6.5 \times 10^{-3}$) at 22 GHz have been achieved with the quartz fibers/urethane acrylate type resin composite laminate material. Therefore, the use of this composite laminate for low loss load-bearing composite panel applications at microwaves becomes totally relevant.

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1:20pm - 1:30pm

Ashes characterization to reduce CO2 emissions

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The operation of thermal power plants for electric energy production implies the generation of heat from coal, oil or other fuels to produce water vapor. The use of fuels produces ashes. Dry and wet fly ash (CSV and CHV) and dry bottom ash (CSF) are by-products of coal power plants and resulting from the combustion of pulverized coal used as fuel. This residue is constituted by the particles that leave the boiler carried by the burnt gases. Ash accounts for 10% of charcoal burned. The grain size of the ashes ranges from 0.5 to 300 micrometers. To avoid pollution, retention is doing before the gas is released into the atmosphere by electrostatic dust separators, and cause large amounts of ash deposited in the land adjacent to power plants. The quality of the ash depends on the fineness, the chemical composition and the mineralogical composition. Silica-alumina ash is produced from bituminous coal and are important because of its pozzolan properties. Sulfur-calcic ashes are produced from lignite and among other minerals have gypsum and calcareous, giving as residue of combustion, calcium sulfate and calcium oxide free. This study offers a promising ashes to reduce CO₂ emissions of greenhouse gases. The results showed that the highest percentage of Ca, O, and C were CSV with respect to CHV, CSF, due higher content of Ca. The analysis by XPS shows possible combinations of Ca2p3 in the presence of the different elements, considering in this case only the C1s, O1s and Si2p, since these resulted bituminous samples as shown in CSF ashes. The CaCO₃ compound was presented in the ashes, as do the studies of XRD and EDS, it has the crystalline structure of compound, and XPS checks that the surface is still present.

Key Words: Fly and bottom ashes, Power plant, Calcium carbonate, CO₂, X-ray diffraction, X-ray photoelectron spectroscopy, and principal component analysis

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1:30pm - 1:40pm

Built-in-Hole a-IGZO p-i-n Diode for Chip-Scale Temperature Mapping

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In this paper, we report design, fabrication and characterization of a vertical built-in-hole p-i-n diode structure using amorphous indium gallium zinc oxide (a-IGZO). The ultimate goal of this design is to use the in-hole a-IGZO p-i-n diode as an accurate on-chip temperature sensor for integrated circuit chips. Since the built-in-hole a-IGZO sensor can be placed right underneath each MOSFET on a chip, it will allow real-time whole-chip temperature mapping with ultra-fine spatial resolution down to transistor level. This novel design opens a door for accurate full-chip thermal management in real time. In this work, a CMOS-compatible process module was developed to fabricate a a-IGZO diode consisting of the following process steps: etching a 10µm deep hole inside a silicon substrate, p-doping in the deep hole to form the p-region, depositing a 10nm aluminum film as the i-layer by atomic layer deposition (ALD), and sputtering to deposit a 150nm a-IGZO layer as the n-region. A a-IGZO p-i-n diode is then formed in the deep hole in the Si substrate. The process module was developed for room temperature to <200°C, hence be compatible to the CMOS back end of line (BEOL) process. DC sweeping test from 0V to 15V across a wide temperature range was conducted for the fabricated a-IGZO p-i-n diode to evaluate its I-V-T behaviors for temperature sensing application. Fig. 1 shows clearly that the built-in-hole a-IGZO p-i-n diode works well and is sensitive to temperature variation. Therefore, the designed built-in-hole a-IGZO p-i-n diode can be used as a temperature sensor to generate real-time full-chip temperature map for power

and thermal management of IC chips.

1:40pm - 1:50pm

Boundary Element Thermomechanical Modeling of Fractional-Order Nonlinear Dual Phase Lag Bio-heat Transfer Problems in Functionally Graded Anisotropic viscoelastic Soft Tissues

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The main objective of this paper is to contribute for increasing development of bio-composites applications according to our boundary element modeling for describing thermomechanical interactions in functionally graded anisotropic (FGA) soft tissues. The governing equations of current model are briefly presented, including the time fractional-order nonlinear dual-phase lag bioheat transfer model and Biot's model. These highly complex governing equations are solved using the boundary element method (BEM), which is an efficient and accurate method for modeling of bioheat distribution in FGA soft tissues, because it only requires discretizing the boundary of the problem, and then dealing with FGA soft tissues problems involving complex shapes. Also, it needs low CPU usage and low RAM usage. The general boundary element method (BEM) based on local radial basis function collocation method (LRBFCM) has been used for solving the time fractional-order nonlinear dual-phase lag bioheat transfer model. Then, the displacement and stress distributions can be achieved by solving the mechanical equation using the convolution quadrature BEM. Numerical results demonstrate the validity, efficiency and accuracy of our proposed modeling technique.

1:50pm - 2:00pm

Effect of Dimensional Parameters on the Mechanical Behavior of Curved Beam Bistable Mechanisms

Lucas Ferreira Lima dos Santos, José Roberto Moraes d'Almeida

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Compliant mechanisms (CM) are vastly studied due to its advantages, such as no need of lubrication, fewer parts and simple manufacturing. Bistable mechanisms (BM) are one of the many types of available CMs. One of the configurations of BMs is formed by connecting two beams at their center, which may be straight or curved beams. This way, a BM can be created and allow applications such as switches, valves, relays, positioners and mechanisms with shock isolation purposes. In this work, a mechanism with a pair of curved beams is used as a model to study the effect of the variation of curved beam parameters on the mechanical behavior of the mechanism. The beam span, apex height and side length were the chosen parameters to be varied, once they are the most relevant to the mechanism design. A comparison was made between the analytical mechanical behavior of the mechanism and numerical approaches, namely, chained beam constraint model (CBCM) and finite element analysis (FEA). It was observed that the side length of the mechanism has major relevance on the bistability condition and the apex height and beam span also play an important role in the force-displacement behavior.

2:00pm - 2:10pm

Nano-enabled multilayer coatings with switchable bacteria-killing activities for prevention of catheter-related infections

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Medical device-associated urinary infections are the most common healthcare related infections accounting for increased morbidity and mortality, prolonged time of hospitalization and huge financial burden on healthcare services. More than 80% of such infections are due to antibiotic resistant biofilm formation, whereas approximately 40% of all hospital acquired infections are catheter-associated urinary tract infections (CAUTIs). Current strategies to reduce CAUTIs include often replacement of the device, which causes considerable discomfort to the patients and increases the treatment costs, or aggressive antibiotic therapies with associated side effects such as hypersensitivity, inflammatory responses and development of drug resistant bacteria. Alternative solutions for effective inhibition of bacterial growth and biofilm establishment on catheters are urgently needed to improve the patient quality of life, safety, and catheters' life-span. In this study, we engineered self-defensive nano-enabled coatings with bacteria-triggered antibacterial activity using layer-by-layer self-assembling approach. Hybrid lignin capped silver nanoparticles (AgLNPs) with high antibacterial activity against a panel of medically relevant Gram-positive and Gram-negative bacterial pathogens were synthesized and used as both functional and structural element in the assembly of the multilayer coatings containing bacteria-degradable elastin and anti-infective/antibiofilm enzyme acylase. The enzyme in the uppermost layer attenuated the virulence of the Gram-negative *Pseudomonas aeruginosa* and inhibited its ability to form resistant biofilms by 90 %, while the triggered release of AgLNPs resulted in total bacteria elimination at lower bactericidal concentrations. These multilayered coatings were biocompatible to human cells and therefore offer potential for addressing catheter related bacterial infections with minimized side-effects.

2:10pm - 2:20pm

Buckling of Functionally Graded Plates Subjected to Partially Distributed Edge Loads

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Buckling behaviour of Functionally Graded Material (FGM) plates subjected to various partially distributed in-plane compressive edge loading is studied using finite element analysis (FEA). The effective material properties of the FGM plates are assumed to vary in the thickness direction according to power-law distribution of volume fraction of the constituents. As the initial pre-buckling stress distribution is nonuniform in nature for a given loading and edge condition, the critical loads are calculated by the dynamic approach. In this study first-order shear deformation theory is used to model functionally graded material plates, considering the effect of transverse shear deformation. Towards this, the plate is discretized by using an eight noded iso-parametric plate element with five degrees of freedom at each node. The analysis is carried out for four types of partially distributed uniform edge compression load, viz., (i) Concentrated edge load from the corner (ii) Partial edge loading at the centre (iii) Partial edge loads from both the ends and (iv) Partial edge load from one end. Convergence and comparison studies have been performed to describe the efficiency of the present model. Solutions obtained from finite element analysis are first validated with results available in the literature for isotropic plates subjected to uniaxial concentrated and partially distributed edge compression loads. Effect of different parameters such as volume fraction index, boundary conditions, modular ratio, side to thickness ratio (b/h), percentage of loaded edge length and edge ratio (a/b) of the plate are considered to study the buckling behaviour of the plate. From the current studies it is concluded that the buckling strength of the functionally graded plate is highly influenced by partially distributed edge loads as compared to plates subjected to uniformly distributed full edge compression. With the increase in the edge ratio, the influence of partially distributed edge load on plate buckling load decreases.

2:20pm - 2:30pm

Additive Manufacturing of Polymer-Derived Ceramic Composites

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Reinforcement of ceramics with a second ceramic phase is a well-established method to create a composite with strength and toughness beyond either constituent material. However, 3D printing approaches that rely on surface interactions for sintering are limited in the amount of reinforcement that can be incorporated. Here we discuss the addition of ceramic reinforcement media to silicon-based, pre-ceramic resins that can be printed on commercial stereolithography printers and subsequently converted into a ceramic matrix composite (CMC) by pyrolysis [1]. We will discuss the use of various reinforcement materials, form factors (e.g. particles and whiskers) and volume fractions in relation to performance and compatibility with the printing method. The CMCs are over an order magnitude stronger and four times tougher than the base polymer-derived ceramic [2]. In addition, we investigate the

high temperature (>1000C) properties of the 3D printed CMCs. Recently we have applied this technology to fabrication of complex packaging for 3D integration of microelectronic subsystems and initial results will be presented

Key Words: Additive, Preceramic, Packaging

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2:30pm - 2:40pm

Bacteriabots - motile “stealth” biological carriers of novel nano-antimicrobial actives

Julio Bastos-Arrieta, Aleksandra Ivanova, Kristina Ivanova, Eva Ramon, Tzanko Tzanov

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The spread of antimicrobial resistant bacteria (e.g. Staphylococcus aureus and Pseudomonas aeruginosa) is a global healthcare concern, reflected in poor treatment outcomes, leading to serious clinical complications, increased mortality, and huge financial burden. During the infection establishment, bacterial cell-to-cell communication process, called quorum sensing (QS), regulates the virulence factors production and formation of antibiotic resistant biofilms via the secretion of highly specific signal molecules. We present a novel micro-transportation system, Bacteriabots, for faster and targeted delivery of antimicrobial actives directly to the site of infection.

These nano-vehicles are composed by a non-pathogenic motile bacteria (carrier) loaded with a nano-enabled cargo entity (e.g. nanoparticles, nanogels) that shows high selective bactericidal efficacy towards Gram positive or Gram negative strains. Our approach would take advantage of the swimming capabilities of non-pathogenic motile human microbiome bacteria. Chemical bonding or electrostatic interactions between the biological carrier and the nano-formulated bactericides will lead to effective formation of the new biohybrid micro-transportation system, in which Bacteriabots driven by Gram positive bacteria will carry the targeted actives against P. aeruginosa and Gram negative carriers against S. aureus. The appropriate cargo and carrier characterization in addition to antimicrobial assays will be presented.

2:40pm - 2:50pm

De Novo Prediction of Light yet Stiff Disordered Atomic Structures by Machine Learning

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The evolution of the Young's modulus (E) of disordered materials (e.g., glasses) as a function of their density (ρ) is typically governed by some scaling laws $E \sim \rho^n$, wherein less efficiently packed structures (i.e., lower ρ) are also less stiff (lower E). The drop in stiffness upon decreasing density is governed by the scaling exponent n , wherein larger scaling exponent results in a more pronounced drop in stiffness. Here, by combining high-throughput molecular dynamics (MD) simulations and Bayesian-optimization-based machine learning (ML), we predict the existence of a “stretching-dominated” family of disordered networks exhibiting minimum scaling exponent. This paves the way toward the design of new ultralight, yet ultrastiff non-crystalline phases.

2:50pm - 3:00pm

Dynamic Behavior of Carbon, Galvanized Iron and Glass Textile Reinforced Concrete Subjected to Impact Loading

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Textile Reinforced Concrete (TRC) has already shown much development as a light weight and thin-walled structural element with high load bearing capacity by evaluating its performance against static loading. Because of its high tensile strength properties, TRCs can be suitable to resist impact loading. Therefore, objective of this research is to investigate the dynamic behavior of TRC under impact loading and to present a comparison of performance between carbon fiber (CF), square oriented galvanized iron fiber (SGIF), diagonal oriented galvanized iron fiber (DGIF) and glass fiber (GF) as textile reinforcement with concrete. Performance of TRC with CF (8 mm opening); SGIF (4 mm opening); DGIF (6 mm opening) and GF (4 mm opening) are evaluated by drop weight impact test method recommended by ACI-544 committee. Total 18 TRC plates of size 300 x 170 mm² and thickness of 25 mm (DGIF and GF), 50 mm and 75 mm (GIF and CF) were tested by dropping an impact load of 4.49 kg from a height of 457 mm with the help of a hardened steel ball of 63.5mm diameter. The number of impact blows at initial crack and ultimate crack were counted and the velocity of the impact load is measured with the help of a high-resolution camera. Performance of the samples is compared by the dynamic and static impact energy. Because of the smaller opening of the fiber fabrics, maximum aggregate size was selected to be 2.36 mm. GI short fiber (0.5% of cement weight) with 0.51mm diameter and 36 mm long was used in concrete. Firstly, 3 TRC plates of DGIF and GF reinforced TRC each (25mm thickness, 1-layer reinforcement) were tested and DGIF textiles showed better results than GF textiles; although the overall performance of both were not satisfactory. Next, SGIF having high tensile properties was taken to compare with another high-performance CF textile. Total 12 TRC plates of 2-layer reinforcement, 3 for each combination (thickness and reinforcement) were tested. For 50 mm and 75 mm thick plates the dynamic and static impact energy of CF is more than 2 times and 1.25 times greater respectively than the TRC with SGIF. Therefore, against impact loading, CF textiles are proved to be the most suitable textile reinforcement; however, SGIF textiles can be an alternative option for CF textiles.

3:00pm - 3:10pm Warning: This presentation lies outside the session time!

Ultrafast laser micro/nano-structured multi-functional carbon fiber reinforced plastic composites for aerospace applications

Dhiraj Kumar, Gerhard Liedl, Andreas Otto, Suhasini Gururaja

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Carbon fiber-reinforced plastics (CFRPs) laminates are extensively used in the aerospace sector due to their high strength and stiffness, low weight, and better fatigue resistance [1]. However, machining-induced damages such as delamination, fiber rupture, fiber-matrix debonding, and high tool wear while using the conventional machining process need to be addressed prior to the usage of CFRPs for various applications [2]. Despite extensive research on replacing metals by CFRPs for weight reduction in aircraft applications, there are open issues such as ice accretion and adhesion that need to be investigated further [3]. Hence, opportunities exist to improve surface characteristics by functionalizing CFRPs using surface micro/nano-texturing [4]. A number of surface functionalization methods have been used earlier such as sol-gel, electrodeposition, lithography, chemical etching, and microreplication. However, ultrafast laser structuring of materials has been accepted as an excellent technique to functionalize the surface [5].

This work focuses on the micro/nano-structuring of the CFRP surfaces using a femtosecond laser. Process parameters were varied to produce laser-induced periodic surface structures (LIPSS) on the material. Melt-free and well-defined hierarchical structures are generated on the CFRP samples that have been characterized using a scanning electron microscope (SEM). Moreover, 3D-optical profilometry was performed to analyze the depth of produced structures. Wettability behavior was assessed by measuring static contact angles (SCAs). Furthermore, treated surfaces were coated with 1H,1H,2H,2H-Perfluorodecyltrithoxy-silane to decrease the surface energy and achieve superhydrophobic behavior. Results indicate a significant increase in SCA along with self-cleaning characteristics after coating. The applicability of laser structured CFRPs surfaces as metamaterials is presently being investigated, and the results would be presented.

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Post-1: Poster Session

Time: Wednesday, 18/Aug/2021: 1:00pm - 3:00pm · Virtual location: Theatre
Session Chair: Monish Chatterjee

1:00pm - 1:03pm

Decoding the Atomic Structure of Cement Hydrates

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Concrete is by far the most manufactured material in the world. However, the atomic structure of its calcium–silicate–hydrate (C–S–H) binding phase remains debated. This arises from the disordered, heterogeneous, multiscale nature of cement hydrates, which prevents the use of conventional experimental techniques to access its atomic structure. Here, we reveal the atomic structure of C–S–H based on force-enhanced atomic refinement (FEAR) simulations. Our atomic model offers an unprecedented description of the structure of C–S–H for varying compositions, both in terms of agreement with diffraction data and energetic stability. An accurate knowledge of the atomic structure of C–S–H is key to accelerate the nanoengineering of novel cementitious binders with enhanced properties or lower carbon footprint.

1:03pm - 1:06pm

Modulation of Mechanical and Luminescence Properties of BORANILs through Sidechain Engineering

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Macromolecule-based organic materials have found wide-spread application in optoelectronics because of their flexibility and tuneable properties. However, small organic molecules lack the mechanical properties needed for device fabrication and require a supporting matrix. Generally, single crystals are brittle and inelastic thereby limiting their use in flexible optical and electronic devices. Flexible organic crystals are emerging as new materials in this direction. Initial advances in this field suggests that a packing pattern consisting of interlocked molecules through weak and dispersive interactions would result in elastically bendable crystals whereas structural anisotropy arising from slip planes leads to plastically bendable crystals.[1] However, it is too early to generalize the design principles because examples of organic crystals that do not follow the above design rules have also been reported. We have synthesized a series of BORANIL molecules by the complexation of Schiff bases with boron (III). Our results indicate that mechanical properties of the molecules can be varied from rigid, brittle crystals to flexible crystals and to organogels through subtle variations in the sidechains. Moreover, the BORANILs exhibited excellent luminescence properties including optical wave-guiding which could further be modulated through supramolecular interactions with entrapped dye molecules.

1:06pm - 1:09pm

Three-dimensional model in assessing the pore geometry of a biomaterial intended for implantation

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Porous biomaterials are widely used in medicine. The right size of pores and connections between them decide about tissue penetration and mineralization, providing a good and durable connection of the implant with the bone. In addition, porous biomaterials are ideal drug carriers because they allow for the placement of a drug substance in the open pores of a biomaterial, and then its introduction directly into the human body during implantation. However, materials with porous structure have to meet strict requirements regarding open and total porosity as well as the size and shape of pores. Various research methods are used to characterize the pore geometry of biomaterials. Most of them are invasive or only allow for the analysis of pores present on the material surface. An alternative to characterizing the geometric structure of material pores is the use of computer modelling and simulation.

The main objective of the study was to develop a three-dimensional model of ceramic biomaterial pores, which would enable to determine the geometric parameters of pores, including their volume. The model creation process consisted of three main stages. The first one involved setting up the assumptions that the model should meet. As part of this stage, measurements were performed using a LEXT OLS4000 confocal scanning laser microscope. The research material consisted of samples of a porous corundum biomaterial produced by chemical foaming. The acquired images were analysed using the Image Metrology SPIP software, which allowed for the separation of pores from the surface image and their measurement. Based on the obtained parameters, the model assumptions were adopted. The next stage was implementation. The model was implemented in the Matlab environment. In order to allow the user to enter the input parameters of the model, a graphical user interface was designed and implemented. The user has the option of specifying the size of the model, the number of pores and the minimum and maximum pore diameter. Based on these parameters, a three-dimensional model is generated. Another element is the possibility of choosing the plane and the position of the cross-section. Based on the model, a computer simulation was carried out, resulting in a three-dimensional representation of the biomaterial pores and its cross-section. By generating the cross-section, the user obtains a flat image of the surface showing the pores located in a given position of the cross-section and in a given plane, as well as the parameters characterizing the biomaterial pores.

1:09pm - 1:12pm

Additive Manufacturing of Polymer/Nanoparticle Composites

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Inventions of new manufacturing methods can innovate down-to-nanoscale material structural control and revolutionize the process of large-scale manufacturing, including logistics and green chemistry. The appearance of additive manufacturing, alternatively termed as 3D printing, is well-known to reduce material waste and be more flexible with complex material design. However, the uses of multiple materials in additive manufacturing has so far been limited to a few polymers and continuous carbon or glass fibers. Our research here reports the uses of 3D printing and how it can include non-continuous nanoparticles in the polymer matrix and manage the location and orientation of nanoparticles. The layer-by-layer assembly can be coherently incorporated on the printing platform so that on the delicately-printed surface morphologies, the nanoparticles can be selectively deposited and oriented. The well-controlled nanoparticle topologies showed anisotropic features that maximized the conductivity along specific axis among all directions. We took advantage of the conductive properties for sensing applications and demonstrated the feasibility in using the manufactured structures for chemical sensors, especially volatile organic compound gases. Our project exhibits the newly innovated manufacturing process and how its autonomy improves the processing efficiency of chemi-resistive sensors.

Topic: Processing and manufacturing technologies

Key Words: additive manufacturing, nanoparticles, sensor

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1:12pm - 1:15pm

Synergistic effect of alginate/BMP-2/Umbilical cord serum-coated on 3D-printed PCL biocomposite for mastoid obliteration model

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Recombinant human bone morphogenetic protein-2 (rhBMP-2) has been used widely in bone tissue regeneration; however, the use of rhBMP-2 can be limited clinically because extremely high doses can cause opposing effects on bone formation, such as high inflammation, edema, and even uncontrollable bone growth. To overcome the limitation of using BMP-2, we used an umbilical cord serum (UCS) that exhibits various growth factors (epidermal growth factor, transforming growth factor- β , nerve growth factor, etc.). To evaluate the effect of the UCS, we studied the synergistic effect of the composite scaffold using BMP-2/UCS/alginate coated on three-dimensional mesh-structured poly-e-caprolactone (PCL), both in vitro and in vivo, using a rat mastoid obliteration model. The newly suggested biocomposite scaffold (BMP-2/UCS/alginate) demonstrates significantly rapid new bone formation (particularly, in the interstitial area of the scaffold) compared to those of two controls: PCL mesh structure coated with alginate, and BMP-2/alginate-coated PCL scaffold. Based on the in vitro and in vivo works, the present study demonstrates that the simultaneous use of low-dose BMP-2 and UCS increases osteogenesis significantly in a rat model compared to the control that uses only BMP-2.

1:15pm - 1:18pm

Atomically Dispersed N-Graphene Quantum Dots-Supported Dinitrosyl Iron Catalyst for Superior Oxygen Evolution Reaction

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The development of robust and non-precious electrocatalysts with high catalytic activity is broadly desired for fuel cell commercialization. Here, we report an electrocatalyst of dispersed Fe(NO)₂ moiety anchored to nitrogen-doped graphene quantum dots (N-GQDs) to form a N-GQDs-Fe(NO)₂ complex that shows a superior oxygen evolution reaction (OER) with a Tafel slope of 47 mV/dec, which exceeds the state-of-the-art RuO₂ (82 mV/dec). Combining X-ray photoelectron spectroscopy and scanning transmission electron microscopy-energy dispersive spectrometer mapping results revealed the catalytically active sites to be monodispersed N-GQDs-Fe(NO)₂ complex that maintain their oxidation state during OER, probably via electronic coupling to the conductive graphene support. Electrochemical data suggest that the Fe-N-C configurations derive their excellent activity from faster OH⁻ adsorption than that of conventional N-C configuration sites. These unique properties of N-GQDs-Fe(NO)₂ complex electrocatalyst could offer a facile route to fabricate non-precious and high OER active electrocatalysts for clean energy applications.

1:18pm - 1:21pm

Effect of Cu and Mn on the microstructure and magnetic properties of $\text{AlNiCoCu}(1-x)\text{FeMn}_x$ high entropy alloy

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It is well known that multicomponent amorphous alloys exhibit excellent soft magnetic properties for high frequency applications. Study of physical properties of multicomponent high entropy alloys (HEAs) is a subject of recent interest HEAs are preferentially defined as alloys containing at least five principal elements, each with an atomic percentage between 5 and 35%. HEAs with a fraction of ferro and non-magnetic elements have been found to show very good soft magnetic characteristics. It has been found that addition of Cu to soft magnetic AlNiCoFe results in phase segregation with magnetically hard phase with saturation magnetization of 84 emu/g and coercivity of 162 Oe. On the other hand, anti-ferromagnetic nature of Mn is inhibited in AlNiCoFeMn HEA as Al changes the Fermi level and itinerant electron-spin coupling leading to ferromagnetism. This has been validated by First-principles density functional calculations on electronic and magnetic structures. It is anticipated that the proper ratio of Cu and Mn in AlNiCoFe can provide superior magnetic properties. In the present work we have investigated the microstructure and magnetic properties of $\text{AlNiCoCu}(1-x)\text{FeMn}_x$ synthesized by Arc melting (AM) and Alloying by mechanically activated annealing (AMAA). Our structural investigations show evolution of ordered BCC phase from mixed BCC+FCC phase with increase in Mn concentration. The highest M_s and H_c for AM samples were 96.6 emu/g and 36.4 Oe for $x=0.75$ and $x=1$ respectively. For AMAA samples the values were 120.4 emu/g and 72.3 Oe for $x=0.5$ and 0.25 respectively. A comparative study of microstructure and magnetic properties of bulk and fine particles will be presented.

1:21pm - 1:24pm

Improvement of magnetic properties and flux pinning for YBCO composites bulk

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Synthesis process of a superconductor can act as flux pinning, resulting in dramatic improvement of magnetic properties. Y_2BaCuO_5 particles can precipitate inside the superconductor, fill up pores, decrease pores, and result in densification of the superconducting microstructure, thereby improving magnetic properties of the superconducting superconductor. The use of additive brought about the control of Y_2BaCuO_5 particles, therefor improving superconducting magnetic properties. When applying the interior seeding technique, the processing period was reduced by half. The top seeding effect was obtained by placing one seed on the upper surface, leading to magnetic levitation force. In order to improve physical properties of superconducting materials, the interior seeding technique was applied and top seeding effect was obtained by placing one seed layer on the top surface. The shape of the top surface of the YBaCuO superconducting single crystal bulk varies depending on the thickness of the specimen. The a-c sector area ratio grows significantly with increasing thickness. The area ratio of the a-c sectors increases but the magnetic flotation of the upper surface decreases. This research was supported by the Korea Electric Power Corporation [Grant number: R16XA01].

1:24pm - 1:27pm

Ferroelectric effect in ZnFe_2O_4 - BaTiO_3 core-shell nanostructures

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Ferromagnetic-ferroelectric ((core-shell) nanostructures are of interest for the single device component with multifunctionality which arises from their strong coupling between ferromagnetic and ferroelectric ordering. Importantly, this type of multifunctional nanostructures will be very useful in various practical applications such as nanoelectronics, magnetic data storage, optoelectronics, and spintronics [1]. We have synthesized ZnFe_2O_4 - BaTiO_3 (2:3) core-shell nanoparticles with a diameter of 60 nm from a one-step polyol method. X-ray diffraction and Raman spectra showed the peaks corresponding to tetragonal BaTiO_3 (BTO) and cubic ZnFe_2O_4 (ZFO) phases. Morphology of the core-shell structure of the calcined NPs at 650 oC is studied using Scanning Electron Microscopy (SEM) and Scanning Probe Microscopy. We found that the BTO shell material grown over the ZFO core due to the lattice mismatch between the ZFO and BTO as ZFO has a large strain value (0.008) with the reduced tetragonality ($c/a = 0.991$). Study of ferroelectric polarization and its domain structure of the ZFO-BTO core-shell NPs are conducted by piezoresponse force microscopy (PFM) in the voltage range from -7 to +7 V with a step of 1 V. The local piezoelectric switching is observed in the BTO shell region at dc bias of ± 7 V. This study also revealed that the core-shell nanostructures are having less ferroelectric polarization in comparison to that of BTO. This is attributed to the encapsulation of the ZFO core within the BTO shell material.

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1:27pm - 1:30pm

Green Mirror-less laser from Conjugated Polymer (PFO-co-PPV-MEHB) in Film

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The purpose of this work is to investigate the optical and mirror-less laser properties of conjugated polymer (CO) Poly[(9,9-dioctylfluorenyl-2,7-diyl)-co-(1,4-diphenylene-vinylene-2-methoxy-5-{2-ethylhexyloxy}-benzene)] also known as [(PFO-co-PPV-MEHB), ADS125GE], in a thin film. The absorption and fluorescence spectra have been measured at various concentrations in toluene. The amplified Spontaneous Emission (ASE) spectra of CO PFO-co-PPV-MEHB in the thin film have obtained at suitable concentrations and pump energies. The pump source was the third harmonic of Nd: YAG laser (355 nm) in transverse mode. The relationship between input pumping energy and output energy for the samples in solutions has been studied. In addition, the photochemical stability of this CO as a laser material was examined. The Time-Resolved Spectroscopy (TRS) studies with the sub-nanosecond resolution have been performed for CO under various pumping energy. These results have provided an understanding of the excited state dynamics of CO PFO-co-PPV-MEHB and have shown that this new CO is quite efficient in the green region under Amplified Spontaneous Emission (ASE) Mode.

1:30pm - 1:33pm

Microbial fuel cell electric power generation

Cirlene Fourquet Bandeira^{1,2}, Mateus Peixoto Oliveira², Diogo Moraes de Souza², Denise Celeste Godoy de Andrade Rodrigues², Gilmar Clemente Silva³, Sérgio Roberto Montoro², Michelle Leali Costa¹, Edson Cocchieri Botelho¹

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Microbial fuel cell (MFC) is a technology that consists of small biological reactors that have the function of converting the energy contained in the molecules of organic compounds into electrical energy or bioelectricity. One of the promising applications of these devices is the treatment of sewage combined with the recovery of energy contained in their molecules. In view of this, the present work aims at evaluating the generation of electric energy in a proton-exchanging membrane "H" (double chamber) type microbial fuel cell, which utilizes the sewage from the sewage treatment plant of the city of Volta Redonda / RJ as its organic source. Experiments have been carried out using the electrochemical impedance and polarization methods to evaluate the generated current and power values. Thus, it can be observed that the system was capable of treating the sewage effectively and produced energy (Maximum current densities = 0.693 mA.cm⁻² and power = 0.693 mW.cm⁻²). Thus, this technology can work to harness the chemical energy of substrates while contributing to water pollution mitigation.

1:33pm - 1:36pm

Development of shuttle adsorbent between the bottom and surface of water for adsorption of pollutants

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For various pollutants having a different specific gravity, the adsorbent having a similar specific gravity to the target pollutant is necessary to achieve enough contact time. Alginate hydrogel composite with controlled specific gravity and/or buoyancy was successfully developed, which can firstly sink in the bottom of water and then float up on the surface of water after the process of adsorption. The purpose of this work is to introduce a self-vertical migration system to the adsorbent for waste water treatment. The alginate hydrogel composite was prepared by using the alginate solution containing both glucose and yeast. The obtained beads firstly sank to the bottom of water, however, 30 min later, most of the beads floated up to the surface of water by generating carbon dioxide in the fermentation. This behavior repeated several times with the fermentation process acted as a float. In order to apply the unique property into the adsorbent, the removal of cesium ions in a water column was demonstrated by using Prussian blue modified alginate gel beads, which have a repeated vertical migration system. As the result, this adsorbent showed the faster removal of cesium than that by the adsorbent without the system. The system can be applied to the treatment of plenty amount of waste water which cannot be stirred and pumping. Therefore, the novel adsorbent developed in this study is expected to contribute to the environmental remediation.

1:36pm - 1:39pm

Edge effects for nonradiative recombination in WS₂

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Transition metal dichalcogenide (TMD) monolayers with direct band gaps are promising materials for various electronic and optoelectronic application. Understanding edge effects and quantifying their influence on the carrier lifetime of monolayer TMDs is fundamental for applying them to high performance electronic and optoelectronic devices. Monolayer WS₂ (tungsten disulfide) with higher photoluminescence quantum yield than other two-dimensional semiconductors (e.g. MoS₂) suggesting relatively low defect density. However, the edge can contain a high density of dangling bonds that can affect the carrier lifetime. Here, we build several possible monolayer WS₂ edge models to simulate edge effects for nonradiative lifetime in monolayer WS₂. These edges introducing trap states into the system can adjust the nonradiative lifetime because of different mechanisms. We are also trying to develop models that quantify the relationship between the nonradiative lifetime and the ratio of the number edge atoms to the number of all the atoms in the model. This study provides a reference for the practical design considering the edge effects for the lifetime of electronic and optoelectronic devices using TMDs from a theoretical perspective.

1:39pm - 1:42pm



Investigation of partial sintering of alumina-containing tetragonal zirconia (ATZ) ceramic composites via temperature-dependent impulse excitation

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Alumina and zirconia ceramics are the most widely used oxide ceramics for many structural and functional applications, ranging from refractory bricks, furnace linings and thermal barrier coatings to transparent ceramics (impact-resistant windows), catalyst supports, filters, fuel cell membranes and biomaterials (bioinert implants). Composites of alumina and zirconia combine the high hardness of alumina with the high strength and fracture toughness as well as the lower elastic modulus (i.e. higher compliance) of zirconia. Moreover, adding alumina to tetragonal zirconia polycrystal (TZP) materials improves the resistance of the latter against hydrothermal aging, i.e. the low-temperature surface degradation due to the tetragonal-to-monoclinic phase transformation, while partial sintering is an easy way to retain porosity in the materials and thus to compensate the increase of elastic modulus (i.e. stiffness) induced by the addition of alumina. Based on extensive experience with impulse excitation measurements of elastic moduli and damping of alumina and zirconia ceramics, both at room temperature and at high temperature (up to 1200 °C), this study investigates the evolution of the elastic properties during partial sintering (during heating and cooling) and the temperature dependence of damping (during heating) of alumina-containing tetragonal zirconia (ATZ) composites (based on Tosoh TZ-3Y20A), prepared by uniaxial pressing and conventional sintering to different temperatures. In particular, the work investigates systematically the evolution of the Young's modulus when the original partial sintering temperature (1000–1400 °C) is exceeded. It is observed that in this case Young's modulus increases concomitantly with the continuing sintering. This work is part of the project "Partially and fully sintered ceramics - processing, microstructure, properties, modeling and sintering theory" (GA18-17899S), supported by the Czech Science Foundation (GAČR).

1:42pm - 1:45pm

Photocatalytic H₂ Generation with g-C₃N₄ and MAI₂O₄ (M=Ba or Mg)

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Photocatalytic hydrogen generation by graphitic carbon nitride (g-C₃N₄) and spinel type MAI₂O₄ (M=Ba or Mg) materials photocatalysts is demonstrated. These are proposed as constituents of a g-C₃N₄ based heterojunction nanomaterial. The g-C₃N₄ photocatalysts were produced by a facile calcination synthesis process of either urea or thiourea. The MAI₂O₄ materials were prepared by combustion synthesis but annealed in air or carbon atmospheres. The characterization of these photocatalysts was done using various methods including X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), Raman Spectroscopy (RS), Brunauer-Emmett-Teller (BET) surface area analysis, Diffuse Reflectance Spectroscopy (DRS), Photoluminescence measurements (PL), and Electrochemical Impedance Spectroscopy (EIS). Their evaluation as photocatalysts in a Hydrogen Evolution Reaction (HER) was carried out under the several irradiation sources including a UV mercury pencil lamp, multiple high-power LEDs (UV-vis range) and visible light LED strips. Triethanolamine (TEOA) was used as the sacrificial agent. A maximum hydrogen generation rate of 97 $\mu\text{mol}\cdot\text{h}^{-1}\cdot\text{g}^{-1}$ was achieved using the carbon annealed magnesium aluminate whilst the urea derived carbon nitride had a superior performance to the thiourea derived carbon nitride. The results further pave way to the fabrication and evaluation of new heterojunction nanomaterials using urea derived carbon nitride and carbon annealed spinel type materials that may enhance the overall photocatalytic performance of either constituent material.

1:45pm - 1:48pm

Recoverable Energy Storage Properties on Pb-based and Pb-free Ferroelectric Thin Films

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Pb(Zr_xTi_{1-x})O₃ (PZT) has been widely used for energy storage applications because of its excellent ferroelectric and piezoelectric properties compared to other ferroelectric materials. The present study describes the influence of rare-earth (RE = La, Eu, Dy and Ho) ions on recoverable energy storage density in PLD grown epitaxial PZT thin films on SRO/LSAT (001) heterostructures. The enhancement of spontaneous polarization in the donor (La, Eu) doped PZT films compared to the pure one is attributed to easy orientation and mobility of domain walls. It is found that the piezoelectric coefficient (d_{33}) is more (130 pm/V) for La doped PZT films (La:PZT), compared to the other rare earth doped PZT thin films. In our results, we found asymmetric polarization versus electric field hysteresis loop and energy storage efficiency (η) values of 30% were recorded in the case of pure PZT film and the value decreased to 28% with Ho doping. However, a high value of 46% could be realized in La:PZT as shown in figure 1. The results will be presented and discussed in details.

1:48pm - 1:51pm

Electropolymerized sorbents for determination of potential endocrine disruptors in environmental samples

Justyna Werner, Robert Frankowski, Tomasz Rębiś, Tomasz Grześkowiak, Agnieszka Zgoła-Grześkowiak

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Several conducting polymers were tested as sorbent materials for the extraction of potential endocrine disruptive compounds from aqueous solutions. Six bisphenols and five parabens were the environmental pollutants selected for this experiment because of their wide range of applications in consumer products [1,2] and presence in the various environmental matrices [3] that can lead to endangering the ecosystem.

The electropolymerized sorbents tested in the study included: polypyrrole, poly(3,4-ethylenedioxythiophene) (PEDOT), and its composite with lignosulfonate (PEDOT/LS). Both sorbents were used in solid-phase microextraction and allowed for the extraction of

bisphenols and parabens from water samples before their chromatographic determination in the LC-MS/MS system. Bisphenols were determined using a procedure with PEDOT/LS sorbent while parabens with the PEDOT sorbent.

Various parameters influencing both methods were optimized including the type of sorbent, time of electropolymerization, preconditioning, extraction time, desorption (time and solvent used), and pH of the aqueous sample. Under optimal conditions the proposed methods allowed to achieve good precision ($n = 5$) ranging between 6.0 and 12.1% for bisphenols and 5.7 and 11.8% for parabens, and recovery levels of 73.8 - 102.8% and 70.1 - 98.0%, respectively. The limits of detection for bisphenols ranged between 0.03 and 0.17 $\mu\text{g L}^{-1}$, for parabens between 0.004 and 0.28 $\mu\text{g L}^{-1}$. The proposed methods were successfully applied for the determination of bisphenols and parabens in aqueous environmental samples giving great selectivity and sensitivity.

1:51pm - 1:54pm

Functional Pickering Emulsion extractant based on Cyanex 923-chitosan-polyethylene glycol for selective extraction of Yttrium from fluorescent lamp wastes

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A novel pickering emulsion (PE) addressed to encapsulate a selective molecule for rare earth extraction (Cyanex 923) into a biopolymer (chitosan) and a non-ionic surfactant (polyethylene glycol 4000, PEG) has been obtained. This PE was applied as extractant emulsion for recovering Yttrium (Y) from a liquid phase containing a blend Y/Ca, which are representative elements of fluorescent lamp wastes after solid-liquid extraction. The PE was obtained by applying ultrasound cavitation in a blend of 30 mL of chitosan of 10 mg/mL, 12 mL of Cyanex 923, and 0.4 g of PEG for 2 min. and 180 W. The PE was characterized by transmission electron microscopy, confocal microscopy, dynamic light scattering, and rheological measurements. The applicability assessment towards Y extraction includes optimal dosage, pH effect, uptake capacity, selectivity, ion strength effect, and reusability tests. 69% of Y was recovered/adsorbed/removed from the Y/Ca mixture with a separation factor ($\beta_{(Y/Ca)}$) of 5. There is not significant impact when the pH and ion strength of the aqueous phase was varied and the material was reused up to 3 times. The PE drop size was 1 μm in average, the distribution of Cyanex 923 into the PE was homogeneous, and the viscoelastic profile of PE showed a long-term stability behavior. To the best of our knowledge, it has been demonstrated for the first time the use of a biopolymer and PEG for encapsulate Cyanex 923 and apply them in rare earth recovery from aqueous phases. This approach offers a broad applicability in the metal extraction, as it would enable to encapsulate other extractant molecules and ion liquids for a desired metal extraction application.

1:54pm - 1:57pm

How the electrode potential selects the dual electronic structure of charged metal-molecule interfaces: Surface-enhanced Raman scattering of cyanide adsorbed on nanostructured silver electrodes

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Experimental and theoretical calculations confirm the existence of two different electronic structures of a surface complex formed by a particular molecule bonded to charged metal electrodes, clusters, or nanoparticles. Each electronic structure of the metal-molecule hybrid system is selected by sign of the surface excess of charge of the metal at potentials more negative or positive than its potential of zero charge (PZC).

Surface-enhanced Raman scattering (SERS) of cyanine adsorbed on a silver electrode shows two regions, which are selected by the voltage and characterized by the differentiated response of the vibrational wavenumbers of the $\nu(\text{CN})$ stretching band. The combination between the experimental SERS and theoretical DFT calculations has allowed for relating the two regions to chemisorbed (C-hybrid, region A) and physisorbed (P-hybrid, region B) surface complexes, where cyanide is bonded through the carbon on top of a single silver atom of the surface. The electrode potential selects one or another type of electronic structure of the system, which are of different nature having a differentiated response to the applied voltage. The electric potential tunes smoothly the wavenumbers, bond energies, and injected charges of the P-hybrid at more negative potentials than PZC, but the very strong C-hybrid prevents significant changes of these properties at positive excesses of charge. The existence of the dual electronic structure of metal-molecule interfaces might require reinterpreting experiments that are usually discussed by resorting to, for instance, the reorientation of the adsorbate, the formation of complexes with different stoichiometries, the existence of nonequivalent local sites on the surface, or to instrumental artifacts. Moreover, this dual behavior also determines the properties and responses of technological devices where metal-molecule interfaces are involved.

1:57pm - 2:00pm

Informing Tunable Bio-composite Design with Fiber Formation in Spiders and Silkworms

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From graphene oxide to polyvinyl alcohol, silk fibroin has been combined with a variety of materials to form composites suitable for a wide range of biological applications. Biocompatible and biodegradable, silk is also extremely versatile – a single spider produces seven different types of silk, each with unique properties such as exceptional strength or extensibility. Creating equally versatile silk composites is of great interest; while micron-sized fibers are an ideal scaffold for nerve repair and regeneration, flexible films provide the perfect foundation for bio-integrated electronic devices. However, though silkworm silk is readily available, industrial scale



synthesis of composites using spider silks is not currently feasible as spiders are cannibalistic and cannot be housed in large quantities. Furthermore, current attempts to produce synthetic fibers have resulted in a material that is inferior to native silk, which boasts the strength of steel and the toughness of Kevlar®. To successfully reproduce this resourceful material and tune its mechanical properties to suit an assortment of bio-composite applications, we must first understand the native silk spinning process.

Though the properties of spider and silkworm fibers have been thoroughly analyzed, there is still a gap in our understanding of how the starting material, a protein-rich hydrogel, develops as it travels down the duct of the silk gland, where it is exposed to shear forces, an acidic pH gradient, and increasing phosphate concentration. In this study, the structural changes in silk protein hydrogels from both spiders and silkworms are analyzed at the atomic, molecular, and mesoscales using a combination of cryo-electron microscopy (cryoEM), Nuclear Magnetic Resonance (NMR) spectroscopy, and Infrared (IR) imaging while mimicking the changing environment within the duct. Replicating the bottom-up, hierarchical assembly of native silk fibers within the duct and understanding how this process affects the mechanical properties of fibers are necessary for developing tunable, synthetic silks that can be integrated into the production of bio-composite materials.

2:00pm - 2:03pm**Investigation on Electrochemical Hydrogen Evolution using different crystal phases of TaS₂****Hamid Ghorbani Shiraz**Linköping University, Sweden; hamgh32@liu.se

Hydrogen has recently been found as the best energy carrier, due to several advantages compared to fossil fuels. Although hydrogen evolution is a relative mature technology, the current production technologies have not met the requirements, e.g., conventional evolution systems have not offered an environmental-safe or energy- and/or cost-effective one. Here, we report an electrocatalyst for evolution of hydrogen which is comparable to the performance of global-standard electrode of Platinum. Electrochemical measurements demonstrates that electrochemical hydrogen evolution at the surface of exfoliated rhombohedral Tantalum disulfide nanosheets, immobilized on surface of glassy carbon electrode using Nafion solution as a binder, is occurred at the significant low overpotential of 0.13 V (Vs. RHE) at 10 mA/cm². However, characterization of the trigonal crystal phase system shows a deteriorated performance toward hydrogen evolution, overpotential of 0.9 V at 10 mA/cm². Investigation of the Tafel plot showed that the slopes for both systems are roughly the same, showing that the kinetically rate of electrochemical reaction and overpotential is comparable for the different crystal phases. Overall, it shows that the structure, which provides the different architecture and configuration of the systems, plays a key role for evolution. It translates that the confinement of sulfur atoms cannot enhance the reduction rate. On the contrary, having the sulfur at the crystal-unit boarder (rhombohedral structure) can increase the efficiency for hydrogen evolution. Higher performance also may be ascribed to the improved diffusion rate of protons toward lattice through exposure of sulfuric sites. It also suggests that hot reaction sites are located on or close to the sulfur atoms. Clearly, electron perturbation arises from heteroatom (sulfur) should also be taken into account. Moreover, calculation of active sites in both systems reveals that the number of active sites in the rhombohedral sample is higher than that of triangle one. It clearly shows that activated basal and edge sites has been formed in the rhombohedral structure.

2:03pm - 2:06pm**Construction and comparison of several different biopolymer coatings on Fe₃O₄ core-shell nanoparticles produced for Doxorubicin delivery.****Maide Gökçe Bekaroğlu, Sevim İşçi**Istanbul Technical University, Dept. of Physics, Maslak 34469, Istanbul, Turkey; bekaroglu@itu.edu.tr

Multifunctional magnetic nanoparticles (MNP) as drug delivery vehicles is a highly researched topic in recent years. Side effects of the used drug could be minimized by accumulating drug loaded MNPs at target site via magnetic manipulations and/or enhanced permeability and retention (EPR) effect. MNPs such as iron oxide nanoparticles (IONP) and their many different formulations are reported to be suitable for drug delivery applications yet there are still several handicaps that needs to be considered such as insufficient accumulation at the target site, toxicity, instability etc. In order to overcome these handicaps, IONPs can be modified to form core-shell structures with biocompatible biopolymers. Biopolymer coatings can modulate physical and chemical properties, improve stability, increase drug loading capacity and optimize drug releasing behavior of IONP core particles. Biopolymer coatings could improve the properties of the core material yet each type of interaction between the drug, polymer and the particle and overall surface charges of core-shell particles could present different outcomes that can affect drug delivery applications. In order to examine these interactions, different types of biopolymers were used to construct Fe₃O₄ core-shell particles for Doxorubicin (DOX) delivery. Polymers were selected depending on their biocompatibility, ionic charges and thermal behaviors. Hydroxyl ethylene cellulose (HEC), nanocrystalline cellulose (NCC), a synthetic biopolymer polyvinyl pyrrolidone (PVP) and κ -Carrageenan (κ -CA) were selected for this study. Fe₃O₄ nanoparticles were coated with each polymer with various concentrations in order to obtain the proper concentrations. Most suitable concentrations were determined via Zeta potential, dynamic light scattering measurements and rheological analysis. Later, for the chosen biopolymer concentrations Fe₃O₄ core-shell particles were further characterized by conventional and in vitro methods. DOX loading capacity determination, in vitro cell viability and drug releasing assays were carried out for every Fe₃O₄ core-shell particle. The results obtained from this study indicated that HEC coated Fe₃O₄ core-shell particle formulation was the most suitable for DOX delivery applications because HEC (a cationic biopolymer) achieved full coverage of the core surface, reduced toxicity to normal cells and successfully loaded and released DOX. On a side note, κ -CA could be a better candidate if the method of drug delivery includes inducing magnetic hyperthermia due to thermo-responsive nature of the polymer, even though the κ -CA coatings displayed decreased drug loading capacities.

2:06pm - 2:09pm**Engineered biomaterials for combination cancer immunotherapy**

James Moon

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With profound advances in immune-oncology, cancer immunotherapy is now considered the fourth pillar of cancer therapy, joining the ranks of surgery, radiotherapy, and chemotherapy. However, only a small subset of cancer patients responds to cancer immunotherapy. While the combination of multiple immune checkpoint blockers generally improves the clinical responses, this can lead to severe immune-related adverse events that result in clinical manifestations of dermatitis, colitis and hepatitis. Thus, new approaches are needed to amplify anti-tumour T-cell immune responses, to convert cold tumours into hot tumours, and to sensitize tumours to immunotherapies with minimal immune-related adverse events. Here, we present new biomaterial-based strategies for amplifying anti-tumor immune responses and sensitizing tumors to immunotherapies in a safe and effective manner. Briefly, we show that lipid-based nanodiscs can efficiently co-deliver antigen and immunostimulatory molecules to draining lymph nodes and elicit potent CD8+ cytotoxic T lymphocyte responses directed against tumor antigens, leading to substantially enhanced anti-tumor efficacy in multiple murine tumor models, including colon carcinoma, melanoma, and glioblastoma multiforme. We have also demonstrated their efficacy in non-human primates. In a second research thrust, we are developing new biomaterials for in situ modulation of the gut microbiome for regulation of local and systemic immune responses. We will share our latest results showing the therapeutic potential of our gut modulation approach in the context of improving the safety and efficacy of immune checkpoint blockers. Owing to the facile manufacturing process, robust therapeutic efficacy, and good safety profiles, our biomaterial-based approaches may offer powerful and convenient platforms for improving cancer immunotherapy and cancer patient outcomes.

2:09pm - 2:12pm

Ultrasound as Functional Influence Tool on FeB pair Association in Silicon Solar Cells

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Defects are crucial for solar cell (SC) performance. The irradiation and annealing are the widespread techniques of functional defect engineering. But another selective as well as room temperature realized way of defects modification is the ultrasound excitation in a crystal. The acoustic waves are able to cause redistribution of impurities, point defects rebuilding and affect SC properties as well [1]. In this work, the influence of ultrasound loading (USL) on a FeB pair association in silicon SC was under consideration. The iron is a major contaminant as well as one of the most detrimental impurities in silicon photovoltaic devices and the investigation is important from an applied point of view.

The Si-SC was fabricated from p-type boron doped wafer with <100> orientation and a doping level of $1.4 \cdot 10^{15} \text{ cm}^{-3}$. In USL case the longitudinal waves with 4.1 MHz frequency and up to $\sim 0.5 \text{ W/cm}^2$ intensity were excited. The FeB pair dissociation was made by halogen lamp illumination (0.25 W/cm^2 , 15 s). The short circuit current value (LED, 940 nm, 0.15 mW/cm^2) was used to characterize recombination process in the SC base. The Isc kinetic was fitted by taking into account intrinsic recombination and to Shockley-Read-Hall recombination on interstitial iron and FeB pair and the iron atom migration energy E_m was determined. The acousto-induced reduction in E_m value has been revealed. The E_m decrease runs up to 10 meV and non-linear depends on US intensity. Thus the ultrasound can be effective tool of defect engineering in solar cell functional materials. The work was supported by NRFU (project 2020.02/0036).

References

1. O. Ya. Olikh, A. M. Gorb, R. G. Chupryna, J. Appl. Phys., 123 (2018) 161573.

2:12pm - 2:15pm Warning: The presentations finish prior to the end of the session!

Rechargeable Magnesium Battery Cathodes Based on Fluorine-free MXenes

Frode Håskjold Fagerli¹, Henning Kaland¹, Jacob Hadler-Jacobsen¹, Zhaohui Wang^{1,2}, Sverre M. Selbach¹, Tor Grande¹, Nils P Wagner^{1,3}, Kjell Wiik¹

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In order for rechargeable Mg batteries (RMBs) to compete with the energy density of today's Li-ion batteries, cathode materials with improved capacity and voltage must be realised.[1] Today's cathode materials suffer from either irreversible intercalation or insufficient energy density, which partly is due to the higher charge density of the divalent Mg-ions compared to Li-ions. One type of material that has been proposed as a possible candidate is the 2D MXene family, where the oxygen terminated vanadium based MXene, V_2CO_x , has shown the highest intercalation energies and lowest migration barriers from DFT calculations.[2] Here, we report on a fluorine-free synthesis route for V_2CT_x MXene ($T = \text{O}$ or OH) by an alkaline etching process. We also show how the material changes by various post-etching treatments. To verify the chemical and structural changes, EDS, XPS, XRD, SEM and Raman spectroscopy are utilized. The effect of the termination groups on the average potential and reversible capacity is experimentally determined and further discussed.

EPMM-2: Electronic, Photonic and Magnetic Materials

Time: Wednesday, 18/Aug/2021: 3:20pm - 6:30pm · Virtual location: AU 2410

Session Chair: Akshay Nagar

3:20pm - 3:35pm

Passive radiative cooling structures for applications in outdoor-useable, patch-type wearable devices

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For wearable devices, thermal management should be provided for accurate signal acquisition as well as thermal comfort. However, outdoor solar energy gain has restricted the efficiency of some wearable devices, resulting in inaccurate data acquisition and skin burn effect [1]. Meanwhile, recently reported passive radiative coolers has been considered as a candidate for an effective cooler with no electricity in many outdoor applications [2-5]. Herein, we present wireless/battery-free and thermally regulated patch-type tissue oximeter (PTO) with radiative cooling structures, which can measure tissue oxygenation under sunlight in reliable manner and will benefit athlete training. To maximize the radiative cooling performance, we introduce a nano-/micro-voids polymer (NMVP) by combining two perforated polymers to both reduce sunlight absorption and maximize thermal radiation. The optimized NMVP exhibits sub-ambient cooling of 6 °C in daytime under various conditions such as scattered/overcast clouds, high humidity, and clear weather. The NMVP-integrated PTO enables maintaining temperature within ~ 1 °C on the skin under sunlight relative to indoor measurement, whereas the normally used, black encapsulated PTO shows over 40 °C owing to solar absorption. The heated PTO exhibits an inaccurate tissue oxygen saturation (StO₂) value of ~ 60 % compared with StO₂ in a normal state (i.e., ~ 80 %). However, our thermally protected PTO presents reliable StO₂ of ~ 80%. This successful demonstration provides a feasible strategy of thermal management in wearable devices for outdoor applications.

3:35pm - 3:50pm

Photon upconversion based on heavy-atom-free thiosquaraines

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Photon upconversion through triplet-triplet annihilation is of interest for a variety of applications, notably as a potential path toward exceeding the Shockley-Queisser limits for solar cells. We demonstrate a completely heavy-atom-free red-to-yellow triplet-triplet annihilation (TTA) photon upconversion system using a thionated squaraine sensitizer, both in fluid solution and in a solid-state composite architecture. Our thiosquaraine exhibits an intense red absorption band, no measurable room-temperature fluorescence, and a native triplet lifetime on the order of 20 μs. This triplet excited state is readily quenched by triplet energy transfer to rubrene as a model upconversion emitter. Selective 685 nm excitation of the thiosquaraine in the upconversion samples results in upconverted rubrene fluorescence centered at 570 nm. The system also exhibits upconversion under filtered red (650 nm long-pass) simulated solar illumination. We also apply this thiosquaraine to demonstrate red-to-yellow photon upconversion in a solid-state polymer composite, a prerequisite for light-harvesting device integration. In contrast with traditional TTA upconversion photosensitizers that require cost-prohibitive precious metals or photodegradable arylhalide groups, we present an easily-tunable squaraine dye that serves as a promising red-absorbing heavy-atom-free upconversion sensitizer for increased scalability and photostability. Our results demonstrate that thionated squaraines provide an exciting new platform for developing heavy-atom-free upconversion systems.

3:50pm - 4:05pm

Surface Plasmonic Sensors for Biomedical Applications: aspects of light-biological matter interaction

Ya-Hong Xie¹, Zirui Liu¹, Tieyi Li¹, Xinke Yu¹, Owen Liang¹, Jun Liu¹, Siddharth Srivastava¹, Yuxing Ren¹, Zeyu Wang², Tony Jun Huang², Feng Li³, Yong Kim³, David T. Wong³

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Surface plasmonics is an avenue of accumulating significant intensity of electromagnetic energy within a small volume of space immediately adjacent to a metal-dielectric (such as air) boundary. When matters such as biofluids are placed within the volume, various processes in the realm of light-matter interaction become possible. One such processes is surface enhanced Raman spectroscopy (SERS). In this report, aspects of the interaction between light and biological matters via Raman spectroscopy are examined from the perspective of diagnostic applications. In other words, what factors of such interaction contribute in which way to the diagnostic efficacy. The report is based on our journey in efforts to establish new diagnostic platforms for several disease types.

The journey began with the fabrication of plasmonic surfaces supplemented with graphene for facilitating quantitative SERS measurements [1]. The nano-engineered surface enabled single-molecule sensitivity and further the manipulation of single molecules via the mechanism of plasmonic tweezers [2]. One aspect of SERS scattering that potentially impact the specificity when studying biomolecules including protein, DNA and RNA comes from the relative orientation of the electric-field and atomic bonds [3]. The level of sensitivity combined with the level of specificity inherent to Raman scattering enabled the use of the plasmonic surface for biomedical diagnostic applications via SERS, a path our research group has followed during the past several years.

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Keywords: SERS; machine learning; exosome; cancer diagnostics;

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4:05pm - 4:20pm

Stretchable Biodegradable Metallic Glass for Transient Electronics

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The recent serious pollution of the soil and ocean by plastic waste provides the lesson that useful and long-lasting inventions sometimes lead to unexpected side effects. The rapid development of electronic devices is now producing excessive electronic waste (e-waste) of toxic or complex materials that are difficult to recycle. In particular, advances in soft and stretchable forms of electronic devices leading the rapid development of biointegrated electronics will bring a severe increase in e-waste. Biodegradable electronic devices are attracting attention as a technology capable of environmentally friendly disposal after their reliable functions are complete. The key idea here -- that even slowly degrading material can be made decomposable in a brief time frame by scaling down material thicknesses at nanoscale -- accelerates the development of biodegradable electronic or transient electronics.

This presentation will spotlight the latest application examples of biodegradable electronics in biomedicine. An amorphous nanoscale metallic glass will be introduced that is both biodegradable and stretchable as an electrode. An electrode of biodegradable metallic glass composed of Ca, Mg and Zn showed elastic strain and fatigue properties superior to those of conventionally structured metals owing to fewer crystalline defects. Integration with other biodegradable layers such as silicon nanomembranes, silicon oxides and PBAT offers various applications in passive and active electronic components as well as a fatigue-resistant triboelectric nanogenerator. Cell toxicity and in-vivo histology results revealed the biocompatibility of this material for use in biointegrated devices.

4:20pm - 4:35pm

Photon avalanching nanoparticles for NIR imaging at 70 nm resolution

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Photon avalanching nanoparticles for NIR imaging at 70 nm resolution

Changhwan Lee, Emma Xu, Yawei Liu, Ayelet Teitelboim, Kaiyuan Yao, Angel Fernandez-Bravo, Agata Kotulska, Sang Hwan Nam, Yung Doug Suh, Artur Bednarkiewicz, Bruce E. Cohen, Emory M. Chan, and P. James Schuck

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Avalanches are steeply nonlinear events in which outsized responses arise from a series of minute inputs. With light, photon avalanching (PA) enables technologies such as optical phase-conjugate imaging, IR quantum counting, and efficient upconverted lasing. However, PA has been observed only in bulk materials and aggregates, often at cryogenic temperatures, preventing its application to bioimaging. We have recently reported the realization of PA at room temperature in sub-30 nm Tm³⁺-doped upconverting nanocrystals and demonstrate their use in high-resolution imaging at wavelengths that fall within NIR spectral windows of maximal biological transparency.¹ Avalanching nanoparticles (ANPs) can be pumped by either continuous-wave or pulsed lasers and exhibit all of the defining features of PA: clear excitation power thresholds, exceptionally long rise time at threshold, and a dominant excited-state absorption that is >10,000 times larger than ground-state absorption. Beyond the avalanching threshold, ANP emission scales with up to the 31st power of pump intensity, an extreme nonlinearity caused by the induced positive optical feedback within each nanocrystal. This enables the experimental realization of photon-avalanche single-beam superresolution imaging (PASSI), achieving sub-70 nm spatial resolution using only simple scanning confocal microscopy and before any computational data analysis. NaYF₄ ANPs with 8-20% Tm³⁺ content can be excited at either 1064 or 1450 nm, with avalanching emission at 800 nm. Pairing the steep nonlinearity of ANPs with existing superresolution techniques and computational methods allows for imaging with higher resolution and at ca. 100-fold lower excitation intensities than is possible with other probes.

1. Lee, C. et al. Giant nonlinear optical responses from photon-avalanching nanoparticles. Nature 589 (2021), 230–235.

4:35pm - 4:45pm

Molecular band THz detection and imaging structures

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Chemical compositions have molecular vibration eigen-modes in THz region and are emitting and absorbing EM waves in this region with wavelengths between 1 mm and 1 mm overlapping in part the thermal emission. The present technology to emit and receive THz waves is bulky and requires complex devices. Integrating conductive microstructures embedded in metal oxides and conducting micro-spheres that creates a voltage parametric amplifier of resonant bands with a FET transistor structure makes possible to create a THz line detector having the size by one order of magnitude bigger than the detected wavelength.

In order to positively identify a molecular species, a plurality of such detectors have to be used together, in order to cover all spectral bands that molecule may emit or not. Supporting the metal structures on piezo-electric materials is possible to tune the resonant frequency of the detector in a larger band and associating several detectors together to be able to scan all THz spectrum producing a direct molecular identification. Further we may tune on a selected substance and using a scanner or a plurality of detection sets to produce a 3D image of the selected substance on a specific timeline, being able to record "chemistry in action".

Because the actual electronics operating frequencies are in GHz domain, at best, and the energy of a THz photon is in meV, it can not be directly detected by photonic devices, we use the perturbation its associated EM wave is inflicting over a differential nonlinear set of FET running a reference signal in GHz or MHz domain, connected to a differential amplifier and a fast, ADC converter connected to a fast direct memory access architecture, shared with a processing computing structure. There are various technological limitations that accounts for various constructive solutions, and the optimization process depends on the application.

Most of the current applications as medicine, chemistry, environment does not require ultra fast imaging and the effort is moved towards the complexity of substances simultaneously present in the area of interest. It has to be noted that THz frequencies have considerably large skin depths in most of materials, except the absorption bands, and in-depth imaging of various bodies may be produced. There is a large palette of applications from security systems to medical, engineering and research systems.

4:45pm - 4:55pm

Better Artificial Photosynthesis by Ion Segregation in Oxide Nanoparticles

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The increase of greenhouse gas in the atmosphere opens an opportunity to use CO₂ and water as a raw material for the manufacture of organic molecules by artificial photosynthesis. Among the different approaches to artificial photosynthesis, the use of semiconductor oxides stands out due to the possibility of generating nanoparticles with large surface areas. However, there is a great challenge to develop nanostructures adapted for the reaction in the gaseous phase, since the solubility of CO₂ in water is limited. Among the different aspects related to the nanostructure of these materials, the construction of surfaces that allow the simultaneous adsorption of water and carbon dioxide is necessary. At the same time, the nanoparticles must absorb light and generate electron-hole pairs with a sufficient lifetime so that the water oxidation and CO₂ reduction can occur satisfactorily. In this case, a large main free path of the electrical charges is important to increase the recombination time that can be improved by increase the conductivity of grain boundaries. Both conditions can be obtained by change the interface composition by segregation of additives during nanoparticles preparation. Segregation is a thermodynamically spontaneous process that modifies the adsorption sites, the depletion layer at the solid-solid interfaces and controls the growth kinetics of the particles. The main propose here is to show how the segregation of additives can be a key factor to prepare semiconductor nanoxides with optimize properties for artificial photosynthesis.

4:55pm - 5:05pm

Composite 3D nanoplatform surface- enhanced Raman scattering and plasmon-enhanced fluorescence detection of serum bilirubin from jaundice

Smruti Ranjan Sahoo, Cheng-Chung Chang, Gou-Jen Wang

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The metal-enhanced fluorescence (MEF) and surface-enhanced Raman scattering (SERS) spectra data can be collected synchronously based on a hybrid 3D-nanoplatform, which is composed of a nanostructure-based substrate and a nanowire-containing solution kit to provides rich "antenna" and "hot spots" effects responding for enzyme free and electrodeless detection of direct bilirubin (d-BLR). The emission enhancement spectra and Raman spectra of d-BLR results were found that the linear detection range is from 1 to 10 μ M with a relatively high R² value of 0.99992, which can be used for detecting abnormal d-BLR concentration from 5 to 10 μ M. The blood serum of MEF and SERS measurement to d-BLR, which can be synchronously collected in one chip, also show linear response ranges with the detection limit as low as 0.5 μ M. The results obtained from our label-free MEF and SERS composite nanoplatform reveals the clinical effectiveness and suitability of the developed in fast-accurate diagnosis of jaundice. Eventually, this hybrid 3D-nanoplatform is worth looking forward to develop as a cheap, robust and portable sensing platform to evaluate the future application.

5:05pm - 5:15pm

Hetero-bimetallic phosphorescent IrIII complexes based on carbene scaffolds and their application in light-emitting devices

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Phosphorescent complexes have been extensively investigated in the last few decades in the fields of organometallic chemistry as well as materials science due to their outstanding photophysical and redox properties.[1] Following the seminal work of Thompson and Forrest,[2] great interest in these classes of photoactive compounds has emerged mainly driven by their application as triplet emitters in phosphorescent organic light-emitting diodes (PhOLEDs). where Ir(ppy)₃-family of complexes (ppy = cyclometalating phenyl-pyridine type of ligands) often represent emitters of choice.[1] On the other hand, NHCs represent an ubiquitous class of ligands in organometallic chemistry since the discovery of stable NHCs[3] The popularity of NHCs stems from the peculiar combination of unique features such as strong σ -donating and relatively weak π -accepting ability and stable M–C bonds, which made them appealing also for designing of phosphorescent emitters.[4]

During the talk, our most recent results in the field will be presented including a novel class of phosphorescent cationic heterobimetallic IrIII/MI complexes, where MI = CuI and AuI where the two metal centers are connected by the hybrid bridging 1,3-dimesityl-5-acetylimidazol-2-ylidene-4-olate (IMesAcac) ligand that combines both a chelating acetylacetonato-like and a monodentate N-heterocyclic carbene site coordinated onto an IrIII and a MI center, respectively. These cationic red-emissive bimetallic species displayed up to two-fold increase of the photoluminescence quantum yield and radiative rate constant compared to the corresponding

mononuclear benchmarks,[5] and achieve record PLQY of 65% for cationic organometallic red emitters. Finally, they successful application as electroluminescent materials in light-emitting electrochemical cells (LECs) will be presented.[6]

Key Words: triplet emitters, iridium emitters, organic light-emitting devices, light-emitting electrochemical cells

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5:15pm - 5:25pm

Quantum dots for two-photon cell transmembrane electric field imaging

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Semiconductor nanoparticles (NPs), more commonly known as quantum dots (QDs) or quantum rods (QRs), exhibit an electric field (E-field) sensitive fluorescence and have been proposed as promising probes for imaging membrane voltages in living cells[1]. Researchers have worked extensively on characterizing the E-field sensitivity of the single-photon fluorescence (1PF) of NPs with a variety of shapes, sizes, and material compositions[2]. And only recently, changes in the fluorescence of membrane-embedded NPs in response to membrane voltages were published[3,4]. In this work, we show that the E-field sensitivity of the two-photon fluorescence (2PF) of type-I and quasi-type-II NPs is more than double with respect to 1PF. Moreover, we have characterized the fluorescence changes in response to transient fields comparable in strength with transmembrane fields in a living cell. Under fast E-field switching, we observe an OFF-transient causing a significant reduction of the fluorescence response to the external E-field, even at frequencies as low as 1 Hz. This severely limits the anticipated performance for the detection of neuronal action. For cardiac electrical activity, however, the impact is limited, and we show that our quasi-type-II QDs can detect a simplified action potential train with an efficiency of roughly 15 % / 60 mV (assuming a 4 nm membrane). These results demonstrate the potential of using QDs/QRs for two-photon action potential imaging in cardiomyocytes.

Figure 1. A) Percentual decrease of the 1PF of 9 nm CdSe/CdS QDs in response to a 400 kV/cm E-field. B) Optical response of the 1PF (top) and 2PF (bottom) to a simulated 30 bpm cardiac action potential train with a ON-level of -150 kV/cm and an OFF-level of 0 kV/cm.

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5:25pm - 5:35pm

Modeling of Magnetorheological gels: A Study on the particle size effect

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Magnetorheological Gels (MRGs) belong to a group of advanced multi-functional materials whose properties can be altered upon the application of an external magnetic field. Usually, MRGs consist of micron and/or nano-sized magnetic particles dispersed in a polymeric gel matrix. Few applications of MRGs include vibration isolation devices, adaptive tuned vibration absorbers, and tunable stiffness actuators.

The mechanical response of MRGs arises from the elastic and viscous contribution of magnetic particles and the polymer matrix, while the magnetic response arises from the interaction between the magnetic particles and the applied external field. In the last two decades, various continuum-based models have been developed to predict this magneto-mechanical behavior of MR materials; however, sometimes, they lack detailed information on the arrangement of particles within the polymer matrix. Hence, a microstructural based approach is adopted to develop a model to study the behavior of the MRGs.

The model developed comprises of the elastic contribution related to the magnetic particles and polymer matrix, the viscoelastic contribution related to the creep or relaxation response of the polymer matrix, the magnetic contribution associated with the interaction between the magnetic particles, and the interfacial contribution linked to the interaction between the particles and the polymeric matrix. The proposed magneto-mechanical constitutive framework is consistent with the thermodynamic framework. Further, the strain energies are developed using the microstructural information of the particle arrangements within the MRGs. This model is utilized to study the influence of the particles' size on the magneto-mechanical behavior of the MRGs.

The developed model is calibrated and validated using a set of experimental data. The results indicate an increasing trend in the modulus value as the particle size decreases under the same volume fraction and magnetic field conditions.

5:35pm - 5:45pm

Multiplexed multi-responsive microneedle hydrogel sensors for chemical analytics useful in diverse applications in Industry 4.0

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Chemical sensors are a major segment of Internet of Things (IoT) devices that are key drivers to the emerging fourth industry revolution (industry 4.0)—that broadly speaking aims to create ‘self aware’ seamlessly interconnected sustainable production ecosystems.

Our research group is focused on developing multi-architecture spectroelectrochemical sensors based on multi-responsive polymers as molecular receptors for multiplex analytes detection. Fabricated by layer by layer (LbL) assembly, in this presentation we will demonstrate our versatile flexible and rigid microneedle electrochemical probes based on biomimetic redox responsive composite hydrogels for in-situ multiplex detection of biologically relevant chemical markers, e.g., dissolved oxygen, redox biomarkers, antioxidants, soil nutrients such as phosphates and nitrates, lactic acid, cortisol, adrenaline, electrolytes, and pH. The composite hydrogels in these sensors simultaneously serves as an interface for biological fluid sampling and a medium for electrochemical sensing. These sensors will be demonstrated as wearable devices, also referred to e-skins, for real-time wireless monitoring of soil/plant growing medium, on-plant plant stress diagnostics, and ‘emotion’ sensing in animals using non-invasive biological fluids, e.g., sweat, and interstitial fluids for animals, and apoplastic exudates for plants. Our embedded multiplex sensors are aimed to be enabling proactive diagnostics technology for realization of environmental, social and economic aspects that align with the United Nation’s Sustainable Development Goals (UN SDGs), particularly sustainable smart agriculture, food security, environmental conservation, and in general equity in global societies wellbeing.

5:45pm - 5:55pm

Partial Leidenfrost Evaporation-Assisted Ultrasensitive Surface-Enhanced Raman Spectroscopy in a Janus Water Droplet on Hierarchical Plasmonic Micro/Nanostructures

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The conventional methods of creating superhydrophobic surface-enhanced Raman spectroscopy (SERS) devices are by conformally coating a nanolayer of hydrophobic materials on micro/nanostructured plasmonic substrates. However, the hydrophobic coating may partially block hot spots and therefore compromise Raman signals of analytes. Here, we report partial Leidenfrost evaporation-assisted fast enrichment of low-concentration analytes in water droplets on hierarchical plasmonic micro/nanostructures, which are fabricated by implanting nanoantennas on carbon nanotubes-decorated Si micropillar arrays. In comparison with natural evaporation, partial Leidenfrost-assisted evaporation provides a levitating force to maintain the analyte droplet in the Cassie-Wenzel hybrid state. In this process, the continuous shrinking circumferential rim of the droplet, which is in the Cassie state, towards the pinned central region of the droplet, which is in the Wenzel state, results in a fast concentration of dilute analyte molecules on a significantly reduced footprint within several minutes. Partial Leidenfrost droplet can reduce the final deposition footprint by 3-4 orders of magnitude and enable ultrasensitive detection of nanomolar analytes because this type of hierarchical plasmonic surface has densely packed plasmonic hot spots with SERS enhancement factors (EFs) exceeding 107. Partial Leidenfrost evaporation-assisted SERS sensing on hierarchical plasmonic micro/nanostructures provides a fast and ultrasensitive biochemical detection strategy without the need for additional surface modifications and chemical treatments.

Key Words: Optofluidics, Nanophotonics, Biosensing, SERS

5:55pm - 6:05pm Warning: The presentations finish prior to the end of the session!

Propyne Hydrogenation over a Pd/Cu(111) Single-Atom Alloy Studied using Ambient Pressure Infrared Spectroscopy

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The hydrogenation of propyne (C_3H_4) to propene (C_3H_6) using a Pd/Cu(111) single-atom alloy (SAA) has been studied using polarization-dependent reflection absorption infrared spectroscopy. This method allows for simultaneous monitoring of reactants and products in the gas phase and species adsorbed on the surface during the reaction. The results were compared with the hydrogenation of propyne using Pd-free Cu(111) as well as with previous studies on Pd/Cu SAA catalysts supported on alumina. Propene production occurs at temperatures of 383 K and above as indicated by the appearance of an infrared peak at 912 cm^{-1} , which is a unique characteristic feature of gas phase propene. Propyne was found to adsorb on the surface at 300 K in the presence of gas phase propyne to form a $\text{di-}\sigma/\text{di-}\pi$ structure, as the spectrum was identical to that reported in the literature for propyne adsorbed on Cu(111) at 150 K in ultrahigh vacuum. The presence of a carbonaceous layer on the surface is indicated by a dramatic increase in the intensity of a peak at 2968 cm^{-1} at temperatures above 400 K. The progression of gas phase peaks at 912 and 3322 cm^{-1} was used to calculate the rate of production of propene and the rate of consumption of propyne, respectively. This reaction rate was used to determine a turnover frequency of 25.4 s^{-1} at 383 K for the reaction on the Pd/Cu(111) SAA surface. The reaction was not impeded by the presence of the carbonaceous layer, even for a layer so thick that only carbon was detectable on the surface with Auger electron spectroscopy.

FCM-2: Functional Composite Materials

Time: Wednesday, 18/Aug/2021: 3:20pm - 6:30pm · Virtual location: AU 2412

Session Chair: Liangbo Liang

3:20pm - 3:30pm

STUDIES ON SYNTHESIS AND CHARACTERIZATION OF NANO-FILMS OF POLYMER BLENDS OF POLY(STYRENE) AND CELLULOSE ACETATE

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The polymer blends are physical mixtures of structurally different polymers which interact with secondary forces with no covalent bonding have assumed a very important status scientifically and technologically. Blending is the process of mixing together of two or more different polymers or copolymers, similar to compounding. Polymer blends offer property, cost and processing advantages and they have been used in an increasing number of application. As cellulose acetate is thermoplastic molding material and biocompatible and used in many industrial and biotechnical applications. Ultrasonic studies have been done by Ultrasonic technique. Characterization of polymeric blends of Poly(Styrene) (PS) and Cellulose Acetate (CA) by physico-chemical, mechanical, SEM, FTIR studies over a wide range of concentrations and temperatures have been discussed to study the degree of miscibility, interactions between the polymer and solvent and polymer compatibility.

3:30pm - 3:40pm

A mass-selective view of local binding and nuclear dynamics in a BaZr_{0.7}Ce_{0.2}Y_{0.1}O_{3-δ} proton conductor as observed by neutron diffraction

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The unique combination of techniques consisting of neutron Compton scattering and neutron diffraction [1-4] have been employed to study a novel proton-conducting system, the hydrated BaZr_{0.7}Ce_{0.2}Y_{0.1}O_{3-δ} (BZCY72), at temperatures between 70 K and 300 K. Neutron data analysis, augmented with density functional theory modelling of lattice dynamics, has enabled a mass-selective view of the combined thermal and nuclear quantum effect on local effective binding. An increased anharmonic character of the lattice dynamics and local binding of the framework atoms is revealed above the orthorhombic to rhombohedral phase transition at 85 K, whereby a subtle interplay between mode hardening and softening with increased temperature tunes the effective local binding of nuclear species. The anharmonic effects seem to be most pronounced in the case of oxygen and cerium. Our analysis strongly suggests the existence of a single type of trapped protons and trap proton sites in the room-temperature non-conducting phase of BZCY72. The protons at room temperature possess insufficiently high kinetic energy to overcome the local barrier for long-range diffusion but enough to perform transfer between different trap sites. Ionic conduction in BZCY72 would then most likely involve two distinct proton types, the ones trapped around the edges of YO₆ octahedra, and the remainder formed of protons located near the ZrO₆ and CeO₆ octahedral edges, the sites that would favour mobile protons. The apparent proton conductivity would then result from a subtle interplay between the population size and mobility of the trapped and free proton fraction as a function of temperature.

Key Words: neutron Compton scattering, neutron diffraction, ab initio lattice dynamics, proton conductors

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3:40pm - 3:50pm

Composite micro-nano-hetro-structures for nuclear power applications

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Nuclear power as we know today has embedded difficulties that finally translated in many accidents and an increase in cost of the energy delivered this way. Main problem is the accelerated degradation of nuclear fuel under the action of fission products, transmutation products and radiation inside the active zone, corroborated with improper temperature distribution and mechanical stress induced during operation.

The searches to solve these problems conducted to development of micro-nano-hetero structures able to use nuclear reaction kinematics to self separate the fission products from the nuclear fuel in microstructures, generically called "Cer-Liq-Mesh", made of nuclear fuel (UO₂, PuO₂, UN, PuN, PuC, etc) micro-beads, with dimensions inside fission products range, chemically stabilized by a thin coating, soaked in liquid metal fluid. In order to assure mechanical stability the micro-beads are suspended on a wire mesh, or felt that is also elastic. As further analyzed, fission products share about 170 MeV in kinetic energy, and in interaction with the matter surrounding the fission origin they behave like charged particles depositing energy as ionization and nuclear recoil towards the end of the stopping range. In solid matter the nuclear recoil zone, also known as Bragg peak is characterized by having many remnant

defects as dislocations. The new solid-liquid composite material, places Bragg peak in liquid, that has exhibits no remnant structural damage.

Transmutation products have shorter stopping range in nuclear fuel in nm range, and in order to extract them, a nano-clustered porous hetero-structure have been developed, where the pores are open and flooded with an extraction fluid, acting as a drain liquid. Nano-cluster exhibit special properties [1] for impurities, different from bulk material, that makes a transmutation product created inside a nano-cluster to be expelled on the boundary from where the extraction liquid washes it out. In an ideal case, the micro-bead may be made of a nano-clustered structure contained inside the coating layer together with the extraction liquid.

This type of nuclear fuel material that contains a porous nano-clustered structure embedded or forming a micro-hetero structure allows the separate extraction of the fission products from the micro-fluid and transmutation products from the nano-fluid may be packed together inside a cladding creating fuel pellet, that may be fully compatible and replace the actual nuclear fuel. The advantage is that after a reasonable burnout, the fission or fission and transmutation products may be extracted on spot and the fuel may be reprocessed pellet by pellet, transferred in a new cladding and used in a breed and burn scheme, reducing the need for enrichment, and by this improving the nuclear fuel cycle and nonproliferation resistance.

3:50pm - 4:00pm

Hysteresis and dielectric properties of functionalized carbon nanotubes - polymer nanocomposite films

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In the recent time polymer nanocomposite films have attracted a great attention to the researchers due to their potential applications in electronic gadgets [1]. Due to semicrystalline nature of some polymers like polyvinylidene fluoride (PVDF) and polyvinyl alcohol (PVA), they are interesting for the applications in electronic device. On the other hand the carbon nanotubes (CNT) have versatile applications in nanoelectronics and they possesses excellent mechanical and electrical properties along with high aspect ratio. The different functionalized (-COOH, -OH, -NH₂) carbon nanotubes (f-CNT)-polymer films are prepared by using an economical and simple solution casting technique [2-3]. Samples are characterized by the X-ray diffraction, atomic force microscope image and two-dimensional fast Fourier transform spectrum analysis, which has confirmed the excellent alignment of f-CNT. The Raman spectra analysis has also confirmed the interaction between f-CNT and polymer and also suggested the formation of p-n junction between them. Hence the f-SWCNT embedded PVA films provide a high dielectric constant at lower f-SWCNT concentration due to their correct orientation. So these films may be used as high-k dielectric films. To illustrate the impedance spectroscopy of the nanocomposite films, we have proposed an impedance based battery equivalent circuit model. The current-voltage characteristic shows a good hysteresis behaviour of the fabricated capacitor of the composite films.

PVDF-f-MWCNT composite films have also shown the temperature dependent current-voltage hysteresis loop, which can be utilized as a non-volatile resistive memory device. To understand the conduction mechanism within the composite films, we have analyzed the measured current density data by using the existing different models. From the analysis, it is observed that during increasing mode of applied field the carrier conduction mechanism follows the Poole-Frenkel model and in the decreasing mode of applied field it follows the Schottky emission model. The trapping and detrapping of electrons takes a significant role in current conduction in this system. The ferroelectric hysteresis loop has been observed and the area under the loops represents the charge storage ability of the pure and composites films. Hence the energy storage density has been enhanced due to high aspect ratio and presence of functionalize group on the surface of MWCNTs and these materials can be utilized to developed polymer-nanocomposites in the field of energy storage application.

Key Words: Polymer, Carbon nanotube, Hysteresis, Dielectric, Energy Storage

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4:00pm - 4:10pm

Empirical mixture rules and their application for estimating the effective conductivity and permittivity of isotropic two-phase composites

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The effective thermal conductivity, electric conductivity or permittivity of isotropic two-phase composites is bounded from above and below by rigorous micromechanical bounds, i.e. one-point (Wiener), two-point (Hashin-Shtrikman) and possibly three-point (Beran) bounds. As long as the phase contrast is small, these traditional contrast bounds provide rather satisfactory predictions, but for large phase contrast the prediction becomes increasingly worse. In this case, mixture rules can be a useful tool to estimate the effective properties, at least when the basic character of the microstructure is known (matrix-inclusion / coated-sphere, bicontinuous or symmetric-cell / granular) or at least to fit measured data for the purpose of meaningful interpolation. The first part of this contribution recalls the classical mixture rules based on the general power mean (which includes, apart from the volume-weighted arithmetic and harmonic means, also non-integer means, such as the Landau-Lifshitz mixture rule), for which a new formulation is given (which also includes the geometric mean or logarithmic mixture rule, i.e. the Lichtenecker relation). In the second part the fixed-parameter weighted means are summarized, which are known under the names Wyllie-Southwick model, Krischer model and Woodside-Messmer model. In the third part special types of floating-parameter means, viz. volume-weighted sigmoidal means, are discussed in some detail. It is shown that only the latter types of means are able to provide meaningful fits (or even rough predictions) for two-phase composites with granular microstructures. Finally it is shown that the volume-weighted sigmoidal means of both Wiener and

Hashin-Shtrikman bounds tend to lie within the Miller bounds for symmetric-cell materials with spherical cells. This work is part of the project "Partially and fully sintered ceramics - processing, microstructure, properties, modeling and sintering theory" (GA18-17899S), supported by the Czech Science Foundation (GAČR).

4:10pm - 4:20pm

Synthesis and Characterization of Titania Pillared Clay Membranes for Methylene Blue degradation in Textile Wastewater

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Textile effluent contains dyes in the range of 50-1000 ppm and at low concentration of 10-50 ppm, thus producing intense colour. According to the Environment Protection Act, these toxic wastes are called 'emerging pollutants' which cannot be degraded by any means. Titania photocatalyst is widely used for degradation of contaminants in wastewater, but its usage suffers from many drawbacks like its ease of separation from the suspension and its tendency towards forming agglomerates which reduces its photocatalytic activity. Amphoteric membranes such as Titania pillared clay membranes exhibit different charges at different pH values, subsequently show efficient separation for cationic and anionic pollutants in wastewater based on solution pH. The structural properties of such membranes determine their permeability and selectivity to a large extent. The present work is envisaged to synthesize TiPILC membranes by immobilizing titania on clay support and further sintered at different temperatures 300degC, 500degC, and 600degC. X-Ray Diffractograms of the membrane material sintered at these temperatures reveal the presence of a mixture of phases, anatase and brookite, responsible for enhanced photocatalysis. Fourier Transform Infra-Red spectra reveal complete intercalation of Ti⁴⁺ ions into interlayer spaces of clay leading to a homogenous material. Brunauer Emmett Teller specific surface area study reveals a narrow pore size distribution curve which reflects the selectivity of the membrane surface. Such a ceramic membrane reactor, an integration of separation along with photocatalysis, when treated with Methylene Blue dye resulted in its ~99% decolourisation in just two cycles of the filtration process.

4:20pm - 4:30pm

De Novo Inverse Design of Nanoporous Structures by Machine Learning

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Nanoporous materials (e.g., zeolite, activated carbon, metal-organic framework, polymeric membranes, etc.) have various technological applications, including gas separation, gas storage, catalytic transformations, etc.^{1,2} The behavior of nanoporous materials (e.g., their sorption isotherm, that is, the amount of adsorbed gas as a function of partial pressure) strongly depends on their pore size and shape distribution. Importantly, the design of new nanoporous materials with tailored structures could enable new breakthroughs in our ability to separate CO₂ from a given flue gas (a prerequisite to CO₂ capture).³ However, our ability to discover new nanoporous materials with tailored functionalities has thus far been plagued by the virtually limitless degrees of freedom involved (i.e., infinite number of potential nanostructures). Here, we present an innovative framework combining high-throughput simulations and machine learning to accelerate the inverse design of nanoporous phases featuring a targeted sorption isotherm.⁴ Our approach consists in (i) hard-coding a lattice-based density functional theory gas sorption simulation as a convolutional network (CNN) in TensorFlow to leverage the automatic differentiation functionalities of TensorFlow (as differentiability simplifies our inverse design problem) and (ii) using this CNN model to efficiently train a deconvolutional network that generates optimal nanoporous structures. This approach enables the de novo design of non-intuitive nanoporous structures featuring unusual sorption isotherms.

4:30pm - 4:40pm

Enzyme-decorated mesoporous silica nanoparticles for elimination of antibiotic resistant *Pseudomonas aeruginosa* biofilms

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Bacterial antibiotic resistance is frequently associated with their ability to form biofilms, acting as a physical barrier that limit the antibiotics penetration and bacterial eradication. Most of the existing strategies aim to inhibit bacterial growth and prevent the biofilm formation, but they become ineffective once the biofilm is well-established. Herein, stimuli-responsive mesoporous silica nanoparticles (MSNPs) were developed for treatment of antibiotic resistant *Pseudomonas aeruginosa* (*P. aeruginosa*) biofilms. In this smart delivery nanosystem, imipenem was loaded inside the pores of MSNPs using high intensity ultrasound and then coated with elastin, which was used as stimuli-responsive gatekeeper degraded by *P. aeruginosa* elastase in biofilms. Subsequently, poly(ethylenimine) and biofilm matrix-degrading enzyme alginate lyase were deposited onto the MSNPs using Layer-by-Layer strategy. At the site of biofilm infection, the enzyme broke down the biofilm matrix and allowed the penetration of the antibiotic loaded MSNPs into the biofilm structure. Then, the *P. aeruginosa* triggered the controlled release of the antibiotic resulting in bacterial elimination and prevention the formation of new biofilm. The developed stimuli-responsive MSNPs exhibited up to 80 % eradication of total biomass and 4 logs bacterial cells viability reduction in already established antibiotic resistant biofilm. These smart MSNPs possess 100% biocompatibility and provide an efficient platform for prevention and treatment of *P. aeruginosa* biofilms.

4:40pm - 4:50pm

Al/Cu laminated wire conductors; effect of stacking sequence on mechanical properties and structural features

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Research and development in virtually all the industrial fields has led to the emergence of numerous modern components, as well as to the introduction of a variety of innovative materials, among which are also modern clad composites [1]. The presented study deals with the preparation of Al-Cu clad composite wires with two different stacking sequences via the intensive plastic deformation technology of rotary swaging (RS). The aim of the work was to provide characterization of the effects of RS on selected structural features and mechanical properties of the composites and their metallic components. The results showed that fine more or less equiaxed grains with no prevailing preferential orientations were present within all the Al and Cu composites' components of the final 5 mm thick wires, which points to the occurrence of dynamic recovery/recrystallization during processing. Grains misorientations were locally present primarily in the Cu components; the Al components did not exhibit any substantial presence of misorientations, which is in accordance with the observed structure relaxation. The tensile tests of the swaged composites revealed both the stacking sequences to exhibit comparable ultimate tensile strength of almost 280 MPa. However, the ductility differed notably; the very low ductility of the composite consisting of Al sheath and Cu wires corresponded to the significant work hardening of the Al sheath, as also documented by the relatively high average microhardness of the Al sheath.

4:50pm - 5:00pm

Buckling and Postbuckling responses of composite plates under combined in-plane loads

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The buckling and postbuckling responses of functionally graded hybrid composite plates subjected to combined in-plane uniaxial compression and in-plane shear loads are investigated numerically. The finite element analysis-based software ABAQUS has been used for the numerical study. Eigen buckling analysis and Tsai-Hill failure criteria are used to determine critical buckling and first ply failure loads, respectively. Functionally graded composite plates with and without cutouts are considered for the study. Five different shapes and three different sizes of cutouts at the center of the plate have been taken to examine the response under the combined in-plane loads. Effect of (0/90)_{4s}, (+45/-45)_{4s}, and (+45/-45/0/90)_{2s} fiber stacking sequences are also examined and load interaction diagrams are presented for combined in-plane uni-axial compression and in-plane positive and negative shear loads. It is concluded that the diamond-shaped cutout of small size among the cutouts performs better in terms of buckling and first ply failure loads of the plates under compressive loads combined with negative in-plane shear load. The (+45/-45)_{4s} stacking sequence has the highest buckling and failure loads in comparison to other layup sequences.

5:00pm - 5:10pm

Electrospinning of PVA/Chitosan/silver nanoparticles, its characterization, and activity on breast cancer

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In this study, we electrospun the Polyvinyl Alcohol (PVA)/chitosan/silver nanoparticle (AgNPs) solution and observed the effect on breast cancer cell line. As silver is known for its anti-cancer properties and anti-inflammatory effect whereas, PVA/chitosan has good fabrication by electrospinning; the combination has prominence in delivery systems. However, in breast cancer, the proposed activity of fabricated material hasn't been well established. To examine this, the silver nanoparticles were incorporated into the polymer solution. Preparation of AgNPs and their analysis was performed to confirm the size and shape of the NPs formed by dynamic light scattering and transmission electron microscope. Further, UV-visible spectroscopy and Fourier transform spectroscopy substantiated the results. We analyzed the morphologies of PVA/chitosan/AgNPs by scanning electron microscope and AgNPs distribution in fiber mesh by mapping the elements. The high aspect ratio of nanofiber tends to allow controlled release of silver and hence related studies were performed. Biocompatibility and cytotoxicity evaluation of nanofibers was done on the fibroblast cells. We performed the in vitro anticancer activity on the breast cell line to prove our concept. This method can be extended through surface modification and conjugation of silver with various biomolecules, peptides, and pharmaceutical active ingredients.

5:10pm - 5:20pm

Production of Sustainable Bio-Composites from Agro-residue Fibers and Recycled Polypropylene

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Wood Plastic Composites (WPCs) have captured a considerable attention in various applications due to their inherent properties like strength and lightweight over conventional polymers. However, using wood as an organic filler for polymers pose a serious challenge to the green areas. Hence, utilization of agro-residues as fillers instead of wood is one of the sustainable solutions to the aforementioned problem. Also, the exploitation of recycled polymers mainly from Municipal Solid Waste (MSW) to produce value added products with economic edge will overcome the adverse impact of polymer waste on the environment. As such, recycling appears to be a valuable future route for sustainable production in polymer-related industries. Thus, research on development of new types of bio-composites prepared using various recycled components is being actively pursued. In this context, our study aims to investigate the potential use of date palm fibers extracted from agro-residue pedicles as a natural filler for synthetic polymers like virgin polypropylene and recycled post-consumer polypropylene. The use of raw and chemically treated fibers is studied and compared. Three levels of fiber content (10 v.%, 20 v.% and 30 v.%) are adopted to manufacture such new class of bio-composites. The influence of date palm fiber content and treatment process on the mechanical and physical performance of the developed bio-composites will be explored. Mechanical testing, hardness, and water absorption of the fabricated specimens are conducted in

accordance with ASTM standards. Fourier Transform Infrared Spectroscopy (FT-IR), X-ray Diffraction (XRD), Thermo-Gravimetric Analysis (TGA), and Differential Scanning Calorimeter (DSC) tests are also performed.

5:20pm - 5:30pm

Formulation and polymerization of Pickering emulsions stabilized by stimuli-responsive dextran-based nanoparticles

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Pickering emulsions offer outstanding kinetic stability, appreciable for storage. It is of great interest to confer them stimuli-responsiveness [1] for applications that often require release of the content. The aim of our work is to formulate Pickering emulsions stabilized by dextran-based stimuli-sensitive nanoparticles. To do so, we modified dextran: a bio-sourced, biocompatible and biodegradable hydrophilic polysaccharide in three different ways. Then, nanoparticles made of modified dextran exhibiting narrow size distribution (PDI<0.2) and average hydrodynamic diameter around 200 nm were produced using nanoprecipitation. The initial modification step provides wettability and ensures stimuli-responsiveness to pH, enzyme or light of these nanoprecipitated particles for their use in Pickering emulsion stabilization. Oil-in-water Pickering emulsions were successfully formulated using these three different types of nanoparticles and limited coalescence phenomenon was studied. Degradation of the nanoparticles and destabilization of the related Pickering emulsions under stimuli (pH [2], enzyme, or light (Figure 1)) were achieved, promoting new bio-friendly vectors for lipophilic substances. The next step is to polymerize the inner phase of simple Pickering emulsions.

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5:30pm - 5:40pm

Hybrid materials obtained from the polymerization of Pickering emulsions stabilized by cellulose nanocrystals

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Cellulose nanocrystals (CNC) are biorenewable particles of rising interest for the stabilization of Pickering emulsions. They are commonly extracted from cellulose substrates, and are needle-shaped nanoparticles (150-200 nm in length, 5-20 nm in width)¹. In the present work, direct, inverted and double emulsions were stabilized using surface modified CNC. Brominated functions grafted bring wettability to the CNC allowing its adsorption at different water/oil interfaces. Taking advantage of this modification, the stabilized emulsions were further polymerized by whether free or controlled radical polymerization leading to objects with a very broad range of morphologies depending on the polymerized phase and initiation locus. The focus was brought on inverse emulsions because very little study was conducted on such systems², as they require modification of the CNC. Solid foams were obtained³ when the polymerization was conducted into the continuous phase while suspension polymerizations of water-in-oil emulsions lead to either full beads or empty capsules. Likewise, elaboration of a new type of capsules (hollow/porous microcapsules) was investigated, by using double emulsions as template and polymerizing their intermediate phase.

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5:40pm - 5:50pm

Interphase characterization of a single glass fiber and epoxy using a tensile test and digital image correlation method

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In this paper, a set-up tensile test for mechanical characterization of glass/epoxy interphase is presented. The test specimens constructed from a single glass fiber embedded in the epoxy resin with the mill scale size. A small testing system is made by the authors in which the tensile test of the specimens can be performed by applying various weights with high accuracy in the range of mg ie.10-5 N and the resulted displacements and strains are measured by digital image correlation (DIC) method in micro or smaller scales.

Using the obtained experimental displacement results for micro tensile tests and by inverse solution of finite element analyses of the specimen, the average interphase mechanical properties can be extracted for glass/epoxy interphase. In this method specimen size is very important and choosing the larger size specimen (similar to standard size) will increase the computational cost or serious difficulties in the problem solving. Therefore, the specimen dimensions should be selected as small as possible.

In the proposed micro tensile test, unlike the nano scale test methods such as nano-indentation, which measure the mechanical properties in a local position, the average interphase properties are calculated along the fiber/epoxy sample interphase, and therefore the obtained mechanical properties are not limited to a specific region of the specimen and preventing the difficulties related to the scattering of results.

The glass/epoxy specimens have a 0.3×0.6 mm cross section and a gauge length of 5 mm. A Canon EOS 6D Mark II camera is used for imaging of tensile tests in DIC procedure. On the surface of each specimen a random pattern of spots is created by spraying paint on the sample. After each test, the taken images are used in an image processing software and the distribution map of deformations and strains are evaluated. The displacement results from this step are entered into the FEM analysis and by performing the inverse solution, an average elastic modulus of the interphase region is calculated.

In another attempt and using DIC, strain distribution on the sample surface are obtained and the effect of interphase region on the strain distribution of specimen is also examined. The authors working on these experimental results to present a variable interphase material characterization as well. More details and results will be presented in the full paper.

5:50pm - 6:00pm

Experimental and numerical damage evolution of polyurethane material using a modified hyper-viscoelastic constitutive model

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Recent investigations about the elastomeric polymer composites emphasized the positive effects of the contribution of elastomers to improve the performance of the protective structures. The unique mechanical and thermal properties and also the self-healing capability of this kind of materials make them remarkable to manufacture highly resilient protective systems. Investigations have shown that the performance of the composite structures with elastomeric polymer coating will significantly enhance their deformation and energy absorption capacity. The nonlinear behavior of elastomers makes major challenge in modeling and investigating the performance of these materials under dynamic loading. This nonlinear behavior caused by the long-chain molecular structure leads to hyper-viscoelastic properties of the elastomers. The characteristics of elastomers depend on different factors such as pressure, temperature and applied loading rate. Therefore, the mechanical behavior of elastomers alters by varying the applied loading rate. One of the most useful elastomers in industrial applications is Polyurethane (PU). PU is a hyper elastic and viscoelastic material formed by isocyanates with chemical reacting of polyol. In this paper several PU specimens made of 3 different shore hardness sheets are subjected to the uniaxial tensile loading to modify the Mooney-Rivlin strain energy density function with a viscoelastic model. The uniaxial tensile tests are also performed for 3 different shore hardness under varying strain rates regimes (between 0.001 to 0.1). Then the numerical model based on the modified hyper-viscoelastic strain density function is developed. For this purpose a user material subroutine is added to the ABAQUS finite element software. Then the analyses are performed to predict the damage evolution and tearing in the PU specimens. The effects of loading rate and shore hardness are also investigated on damage evolution of the polyurethane material under dynamic loading.

6:00pm - 6:10pm Warning: The presentations finish prior to the end of the session!

Soft and highly sensitive capacitive pressure sensors array based on a polymeric foam

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Flexible low-pressure sensors have raised a lot of interest in the past ten years for their promising applications in health [1] (such as biomonitors and electronic skin) but also as tunable electronic devices that could be used both in sport and industry [2]. We present here an unconventional capacitive pressure sensor, based on a polymeric foam filled with conductive carbon black particles. We design a new material by preparing a PDMS porous material of closed porosity by using an emulsion road [3]. The surface of the closed pores is covered by carbon black conductive particles. These materials have very high permittivity

($\epsilon_r=1000$ at 10 Hz) and display large electrostrictive coefficient. The sensors made by using these materials are low-cost, highly sensitive at low pressures ($S = 5 \text{ kPa}^{-1}$ for pressures $< 1 \text{ kPa}$) [3] and particularly versatile. We show that they can easily be built in arrays of varying shape and size with a simple adaptation of the bottom electrode, and their sensitivity is tuned by varying the thickness of the polymeric foam and their geometry. In particular, we build a $4 \times 4 \text{ cm}^2$ array of 25 sensors, and use it to measure the small ($< 500 \text{ Pa}$) and localized pressures which develop in the flow of complex fluids. The sensors are placed either on the plate of a classical rheometer, or used to measure the forces arising during the spreading of a liquid on a soft substrate. We demonstrate that pressures as small as 5 Pa can be easily detected, which allows us to build a 2D mapping of the local pressure. Beyond obvious applications in industry, the versatility of our devices make them particularly promising in sports, for example for smart shoe insoles.

Key Words: Low-pressure sensor, flexible electronics

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FESC-INV-1: Functional Materials for Energy Storage and Conversion Devices

Time: Wednesday, 18/Aug/2021: 3:20pm - 7:20pm · Virtual location: Theatre

Session Chair: Elham Sahraei

Session Chair: Muhammad Imran Shakir

3:20pm - 3:35pm

Cationic and Anionic Redox Chemistry in Oxide-Based Battery Cathodes

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The pressing demand of high energy batteries for modern energy applications calls for clarifications and optimizations of the redox chemistry involved in battery operations. As the bottleneck of battery energy density, oxide-based battery cathodes suffer complicated issues of the involvements of both the transition metal (cation) and the oxygen (anion) in the redox reactions during the high voltage cycling, which relies on modern characterization tools to reveal the underlying chemistry and guidelines for optimizations.

This presentation introduces recent developments and studies of oxide cathodes through advanced soft X-ray spectroscopy, especially resonant inelastic X-ray scattering (RIXS) in the soft X-ray range of the oxygen (K-edge) and transition metals (L-edges)[1]. We discuss several demonstrations on Li-ion and Na-ion battery cathode studies[2], and provide our spectroscopic views on the TM and Oxygen redox behaviors in Li-rich and conventional cathode compounds[3], which are directly related with some critical issues, such as stability[4] and kinetics[5], in batteries operated at high voltages.

Key Words: Battery, Cathode Materials, Redox Mechanism, Soft X-ray Spectroscopy, Oxygen Redox Reaction

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3:35pm - 3:50pm

Ultra-thin Electrodeposited Noble Metals Layers on Max Phases Based Support for Green Energy Production

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Ultra-thin Electrodeposited Noble Metals Layers on Max Phases Based Support for Green Energy Production

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Hydrogen is considered as pure, high conversion efficiency fuel for prospective application in environmental friendly power sources. Pure hydrogen could be produced by water electrolysis. However, the main problem for hydrogen fuel production is still high energy consumption (~5 kW m⁻³ of H₂). Thus, development of high efficiency catalysts for water electrolysis is still remained. We have established simple electrochemical method for deposition of thin layers of noble metals – Iridium and Platinum on Ti₂AlC and Nb₂AlC supports, respectively [1]. Namely, only several nanometers thick layers of noble metals were deposited and investigated as the cathode catalysts for hydrogen production in acid solutions. The synthesized catalysts exhibited high performance especially at industrial electrolysis working conditions, e.g. at high current densities (-0.3 A cm⁻²). Having in mind extremely high chemical stability, high conductivity and low cost production of Max phases based supports these novel catalysts could be considered as promising for efficient green energy production.

Acknowledgement: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-68/2020-14/200053). Special thanks to Prof. M. Radovic from the Department of Materials Science and Engineering, Texas A&M University, College Station, TX 77843, USA, for preparation of Ti₂AlC and Nb₂AlC substrates.

Key Words: Keywords: Hydrogen production, Electrodeposition, Ir and Pt layers, Max Phases, acid solution

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3:50pm - 4:05pm

Developing Multifunctional, High Performance Thiazolothiazole Materials for Electronic and Optical Applications

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Thiazolothiazole (TTz) materials are promising molecular platforms for a variety of electronic and optical applications. We have developed TTz dye systems that can serve as an electrochromic material, (1) as a dye for biosensing applications, (2) and as a stable material for molecular electronics and energy storage. Extended TTz viologen structures demonstrate both reversible electrochromic behavior and high fluorescence quantum efficiency that is deactivated with electrochemical reduction. Water-soluble, chromogenic TTz derivatives show excellent reversibility and stable cycling in a simple aqueous, polyvinyl alcohol/borax gel electrolyte electrochromic device. They produce voltage-dependent purple or blue coloration and efficient electrofluorochromism. We have also developed environmentally sensitive asymmetric TTz derivatives can serve as molecular probes for cell imaging and cell membrane voltage sensing. These asymmetric TTz derivatives exhibit strong solvatofluorochromism with fluorescence quantum yields > 0.9. In vitro cell studies indicate good cell membrane localization, insignificant cytotoxicity, promising voltage sensitivities, and photostability that is 4 times higher than comparable dyes. Lastly, solution-processable TTz compounds can be used as charge transport layers in a variety of molecular electronic devices (OLEDs and OPVs) and as energy storage materials. Their ease of synthesis and purification, remarkable photophysical properties, and chemically sensitive TTz bridge make these materials attractive for multi-functional optoelectronic, electron transfer, electrochromic, and other photochemical / energy storage applications.

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4:05pm - 4:20pm

Nanoscale Function in Perovskite and Organic Solar Cells

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Perovskite and organic solar cells are promising for enabling low-cost solar energy harvesting, while offering a lightweight and flexible form factor. Despite stunningly rapid progress in the performance of organic-inorganic lead halide perovskite solar cells, the causes of local spatial heterogeneities in photovoltaic properties remain poorly understood. For organic solar cells, the nanostructured interpenetrating donor-acceptor active layer required for high performance operation poses a challenge for disentangling the effects of nanoscale structure on optoelectronic processes. In this talk, I will outline our recent efforts to unravel nanoscale structure-function links in these emerging photovoltaic systems. Using point-by-point current-voltage mapping based on conductive atomic force microscopy [1], we observed an enhanced open-circuit voltage and suppressed short-circuit current near grain boundaries in methylammonium lead halide perovskite active layers. Nanoscale nonlinear strain and surface potential mapping provide evidence for field-induced methylammonium cation buildup and band bending near grain boundaries that reduce charge carrier recombination, but may trap charge [2,3]. Nanoscale point-by-point current-voltage mapping of hole mobility in bulk heterojunction organic solar cells highlights the importance of in-plane charge transport pathways for facilitating out-of-plane charge flow [4,5]. This conclusion is bolstered by data that shows improved charge percolation when there is balance of crystallite orientations. These experiments highlight the significant role of nanoscale structure in emerging photovoltaic systems and the importance of co-localized nanoscale structure-function analysis to unlock the potential of new photovoltaic materials.

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4:20pm - 4:35pm

Theoretical Optimization of bi-facial BIPV Module for Apartment

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Theoretical Optimization of bi-facial BIPV Module for Apartment

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There are many kinds of technologies to mitigate greenhouse gases for a sustainable world. The largest portion of greenhouse gases comes from the building sector, especially in developed countries. In Korea, all new public buildings (Total floor area: 1,000 π^2) by 2020 and all buildings (Total floor area: 500 π^2) by 2030 should be built as a near-zero energy building to mitigate greenhouse gases in the building sector. The theme of this research is to ecologically supply nearly zero-energy solar architecture with minimal cost by

suggesting the optimal energy harvesting methodologies, multi-functional BIPV, reasonable building envelope concepts, considering the regional climate and architectural culture of the corresponding climate zone combined to bi-facial BIPV module system.

This research is mathematically analyzed to make an ecological PV envelope system or design criteria close to a zero-energy building, as a kind of multi-functional building integrated photovoltaic (BIPV) which bi-facial BIPV modules are deployed to passive solar concepts, to minimize the heating & cooling load, to upgrade the indoor environmental quality, and to be adjustable for regional climate, and to continuously succeed architectural culture and history through optimization of element technologies including any possible system based on natural energy resources, to fundamentally mitigate climate change and indoor environment.

The concept and design criteria for the nearly zero-energy solar architecture of this research are focused on the ecological use of bi-facial PV modules. How to maximize solar gain in the heating period, how to eliminate solar irradiance outside the building envelope in the cooling period, and how to maximize power generation by bi-facial BIPV module could be the most important interest for this research. This multi-functional BIPV concept of bi-facial PV module as a shading device could be also ecologically nice PV technology with the passive intelligent system concept in an eco-friendly and effective manner while improving the human comfort in a building and drastically reducing the cooling load of a building, especially in a hot or temperate climate zone.

Key Words: Passive intelligence, multi-functional BIPV, Bi-facial PV module, Building energy conservation.

The author acknowledges the financial support of Sehan University.

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4:35pm - 4:50pm

Thermodynamic interpretation of the open-circuit voltage in energy conversion materials

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Renewable energy converter, such as solar energy converter or thermoelectric converter, are inherently nonequilibrium systems. For example, the driving force in solar energy converter is given by the illumination. The performance of solar cell operation can be assessed by the efficiency that relates the useful output power to the total power incident. The useful output can be interpreted as the work against an applied load and the current-voltage characteristic of a solar cell represents all possible working points as function of the voltage (applied load). The discussion of fundamental limits to photovoltaic efficiencies, the enhancement of power conversion efficiencies, and efficiency forecasts has been guided the research activities in the field of renewable energy conversion. Efficiency limits can be obtained by thermodynamic arguments, for example, when looking at the zero-power operation of a solar cell or when looking at the maximum power point. The zero-power limit of a solar cell is given either under short-circuit operation, $J_{sc}(V=0)$, or under open-circuit operation. The open-circuit voltage defines a stopping point V_{oc} at which the applied voltage stops the current, i.e., $J(V_{oc})=0$. Focusing on state models for bulk heterojunction organic solar cell that includes the essential optical and interfacial electronic processes, we show that the open-circuit voltage is a special thermodynamic equilibrium point, at which the state occupation probability is given by Gibbs-like distribution. The Gibbs-like distribution which can be used to calculate both the entropy of the stopping configuration and the entropy of the equilibrium reference state. An interesting quantitative measure of the difference between the stopping configuration and its associated "true" equilibrium configuration is given by the so-called relative entropy or Kullback-Leibler entropy (divergence). The Thermodynamic interpretation of the open-circuit voltage provides a framework to calculate analytically the open circuit-voltage in dependence on the underlying microscopic processes. This study offers a promising route to include different types carrier recombination processes and discuss its consequence on the open-circuit voltage.

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4:50pm - 5:05pm

Intermediate-temperature solid oxide fuel cells: Fabrication on porous metallic supports. Impregnation of CGO-backbone electrodes for SOFC application.

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Intermediate-temperature solid oxide fuel cells:

Fabrication on porous metallic supports.

Impregnation of CGO-backbone electrodes for SOFC application.

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Solid oxide fuel cells (SOFCs) are promising devices for energy-conversion applications due to their high electrical efficiency and eco-friendly behavior [1-2]. Their performance is not only influenced by the microstructural and electrical properties of the different layers of the unit cell, i.e. electrodes and electrolyte [3]. Indeed it also depends on the interactions at the cathode-electrolyte and anode-electrolyte interfaces [3-4]. Nowadays, commercial SOFCs are electrically efficient at high operating temperatures, typically between 800 and 1000 °C. This high-temperature range restricts their real-life applications, but also their lifetime. Our basic goal deals with the objectives to reduce the operating temperature by working in the range from 500 to 700 °C, and to develop low-cost IT-SOFCs. In the present work, we have elaborated metal-supported solid oxide fuel cells (MS-IT-SOFCs) that would provide very cheap SOFC cells with increased lifetime and reduced operating temperature.

Recently our work focuses on the physical, chemical and electrical characterizations of porous CGO-backbone cathodes which have been impregnated with a LSCF sol-gel solution. The porosity of the backbone was controlled by the addition of different pore-formers. We have demonstrated an important effect: whatever the temperature, from 500 to 700 °C, the cathode resistivity can be tuned both by the LSCF solution viscosity and by the kind of pore-former.

Key Words: CGO, LSCF, pore-former, oxide, cathode, SOFC.

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5:05pm - 5:20pm

Poly-ynes, Poly(metalla-ynes), Coordination Complexes and Polymers for Opto-Electronic (O-E) Applications

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The quest for high performance opto-electronic (O-E) devices for sustainable energy have led to the development of new generation efficient, cost-effective, and lightweight solar cells (SCs) and organic light emitting devices (OLEDs) based on conjugated organics, organometallics, coordination complexes and polymers.¹ This has been possible largely due to the diverse modern synthetic protocols generating new functional materials with easily tunable properties such as extended π -conjugation, good absorption profile, photoluminescence (PL) etc. A wide range of conjugated organic, organometallic and coordination polymers as well as their model compounds are extensively investigated in our laboratory (Chart 1). The first series consists of Pt(II) poly-ynes incorporating a wide variety of conjugated carbocyclic, hetero-cyclic and mixed hetero-cyclic spacers. Pt(II) poly-ynes are excellent phosphorescent materials with long-lived triplets promoting charge generation and enhancing efficiency of the O-E devices. The second series is comprised of organic co-polyynes using phenothiazine (PTZ) as a common motif. The materials have shown promise for application in bulk hetero-junction (BHJ) SCs and polymer LEDs. The third series is comprised of metal organic framework (MOF) materials, self-assembled from ferrocenyl ethynylpyridine and Cu(I) halides. A range of dinuclear aryethynylpyridine Cu(I) halide phosphine complexes (aryl = carbocyclic and heterocyclic spacers) bearing anchoring carboxyl acid groups have been assessed as dyes in DSSCs. The fourth series consists of luminescent coordination complexes of trivalent lanthanide ions. The complexes have been utilized as emitting layer in the OLEDs to fabricate red, green and even white OLEDs. The design, synthesis, chemistry and photophysics of these materials will be reviewed with structural analysis of their model compounds. Fabrication of SCs and OLEDs incorporating these novel materials and evaluation of their device performance will be presented.

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Members of the Materials Research Group

Prof. Paul R. Raithby, Dr. Nawal Al-Rasbi, Dr. Mohamed Al-Suti, Dr. Rashid Ilmi, Dr. Ashanul Haque.

5:20pm - 5:35pm

Towards Mimicking Light-Harvesting Organelle Function with Water-Soluble Conjugated Polymers

Alexander Ayzner

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The ability to assemble complex, artificial light-harvesting systems that mimic natural light-harvesting organelles in water is both fascinating and attractive from a practical point of view. The components of such a system must be capable of self-assembly and strong light absorption. They must also support rapid transport of photogenerated electronic excited states (excitons) through space to ensure that few photons are wasted. Excitons must then be converted to electron/hole pairs that live long enough to drive chemical reactions. Conjugated polyelectrolytes (CPEs) combine several characteristics that make this materials class a promising foundation for this application. Using these materials, we are focusing on associative phase separation of CPEs as a means to form membrane-less light-harvesting organelle mimics. We have shown that associative phase separation can form complex coacervate-like concentrated CPE fluids with photophysics that can be manipulated with simple ions via the cation- π interaction. Our recent work shows that molecular ions can stabilize concentrated phases that contain an exciton donor/acceptor CPE network with properties

reminiscent of dense fluids and hydrogels. In parallel, we are also working on constructing hierarchical membrane-based panchromatic systems based on soft macroion vesicle scaffolds. To form an exciton and electron cascade that forms long-lived electron/hole pairs, we aim to simultaneously take advantage of both the outer and inner membrane/water interfaces, along with the hydrophobic membrane interior. I will discuss our current progress in forming self-assembled, directional exciton funnels oriented from outside towards the membrane interior.

5:35pm - 5:50pm

Design of Materials for Advanced Energy Storage

Cengiz Sinan Ozkan

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The global electrochemical energy storage market ranging from electric vehicles and personal electronics to physical grid storage and defense applications demands the development of new classes of materials for fabricating high performance batteries and supercapacitors. I will describe innovative approaches for the design and synthesis of nanostructured materials towards enhanced reversible capacity; superior rate performance and cycling stability; superior gravimetric capacitance; and enhanced energy density and power density. Hierarchical three dimensional (3D) graphene-carbon nanotube hybrid materials called pillared graphene nanostructures (PGN) grown by chemical vapor deposition possess ultra large surface area, tunability, mechanical durability and high conductivity which are appealing to diverse energy storage systems. Integration of nanostructured pseudocapacitive metal oxides to such 3D hierarchical templates provides superior electrochemical performance. Among the high performance capacitor systems developed includes MGM (graphene-MWNT-Manganese oxide) and RGM (graphene-MWNT-Ruthenium oxide) hybrid systems. High specific/areal capacitance and extended operational voltage window provides an exceptionally high energy density and power density. Similar three-dimensional templates are transformed into cone-shaped carbon nanotube clusters decorated with amorphous silicon for lithium ion battery anodes (SCCC), by depositing amorphous silicon onto the mesoporous nano-carbon templates via magnetron sputtering. The seamless connection between silicon decorated CNT cones and the graphene substrate facilitates charge transfer and provides a binder-free technique for preparing lithium ion battery anodes. Lithium ion batteries based on the SCCC architecture demonstrated ultra-fast charging, high reversible capacity and excellent cycling stability. Mildly reduced graphene oxide (mrGO) and silica coated Sulfur particles (SCSP) have been developed as new generation cathode materials, forming the basis for Li-S batteries. During cycling, SCSPs fracture and release active material, and mrGO helps to contain the ruptured particles, thereby reducing the polysulfide shuttling effects and improving the cycling stability. In addition, I will describe the use of computerized tomography (CT) scans for physical characterization of batteries. Selected metal oxide (MO₂) thin film barrier layers have been developed to further mitigate the polysulfide shuttling effects, and to further enhance the performance and cyclic stability of Li-S batteries. Through analysing the binding energies of Li₂Sn adsorbed onto selected MO₂ surfaces via density functional theory (DFT) calculations and Molecular dynamics (MD) simulations, we show that the strong Li-O bonds dominate the interactions between Li₂Sn and selected MO₂ surfaces. Our studies demonstrate that selected MO₂ thin film barrier layers could be employed to further enhance Li-S battery performance.

5:50pm - 6:05pm

Chemically Bonded 3D Porous Network of Black Phosphorus@MXenes Enables High and Stable Capacitive Energy Storage

John Wang, Zhenghui Pan

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The performance of supercapacitors is largely limited by the lack of high-mass-loading electrodes (~10 mg cm⁻²) and therefore they offer relatively low volumetric energy density, where there is an increase in limit of ion diffusions with thickening in film electrodes. We have developed a rational design for black phosphorus@MXenes compact films of 3D chemically bonded porous network structure. They are successfully made by in-situ growth of black phosphorus (BP) nanoparticles on 2D MXene, and give rise to a commercial-level capacitive energy storage at high mass loading (>10 mg cm⁻²). The strong chemical bonds (Ti-O-P) formed between BP nanoparticles and 2D Ti₃C₂ stabilize the 3D porous network structure, and therefore enable sufficient charge transports and electron environment for electrolyte ions absorption and storage. The 3D network porous structure formed by incorporation of BP nanoparticles into 2D MXene further facilitate highly reversible ion adsorption reactions that contribute fast charging/discharging capability. The BP@Ti₃C₂ compact film electrode delivers an impressive volumetric capacitance of ~350 F cm⁻³, which is among the best performance ever reported so far for MXene-based SCs employing ionic liquid electrolyte. The supercapacitors made use of the BP@Ti₃C₂ compact film electrode with a mass loading of ~15 mg cm⁻² offers a high stack volumetric energy density of >70 Wh L⁻¹. We have conducted thorough investigations into the rationally designed 3D porous network structure of BP@Ti₃C₂ with chemical bonds between the two, and the key working principles are revealed.

6:05pm - 6:20pm

Electrochemical production of high-purity silicon in molten salts towards energy-related applications

Xingli Zou, Xiongqiang Lu

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Crystalline silicon solar cells have dominated the photovoltaics (PV) market for the past several decades and are most likely to continue to be the primary technology for the PV industry in the future due to its abundant raw materials supply and non-toxicity. One of the long-standing challenges is the high-purity silicon production cost because of its complex and energy-intensive production processes. In addition, nanostructured silicon as electrode material also has great potential for energy storage applications. However, cost-effective production of high-purity silicon materials still remains a challenge. The molten salt electrochemical process provides a

possible alternative route for the cost-effective production of silicon for various energy-related applications. In this work, we present the demonstration of electrochemical production of high-purity silicon materials with different morphologies in molten salts. Silicon materials with tunable morphologies, i.e., dense silicon films, silicon nanowires, silicon particles were produced in a controlled manner in molten salts, and the reaction mechanisms involving an in-situ dissolution-electrodeposition process were systematically investigated. This study offers a promising route to facily produce silicon materials for various energy-related applications.

6:20pm - 6:35pm Warning: The presentations finish prior to the end of the session!

Modelling Damage in Grain Engineered Voids, Precipitate and Microstructural Distortions during 3D Printing Process

Frank Abdi¹, Amir Eftekharian¹, Dade Huang¹, Kamran Nikbin², Yun Hu²

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Additively Manufactured (AM) parts exhibit cracks, low toughness, low plasticity, and high residual stresses. To mitigate these characteristics, a process for grain microstructure in AM alloys is desirable. Integrated Computational Material Engineering (ICME), tools can guide the AM process and predict thermo-mechanical, fracture-fatigue behaviour and altering the process parameters to predict microstructural change. Furthermore, the modelling is needed to predict effect of defects, and inclusions effect on mechanical properties that are important to take AM to mainstream component applications. The microstructures resulting from 3D printing processes of engineering alloys are complex in nature and are effectively the result of micro-welding processes which leave, voids, precipitates, distorted grains, and residual stresses in the process. The 3D techniques are being continuously developed to improve creep/fatigue and oxidation strength of components. Furthermore, these more complex microstructures due to the new fabrication methods mean that a whole new approach is needed in the material testing verification as well predictive modelling to optimize both the laboratory testing and operational processes in components. In this effort grain boundary engineering (GBE) multi-scale modelling of stainless steel is performed to expedite qualification process for existing and new AM polycrystalline alloys. ICME develops a procedure for a meso-scale grain/grain boundary engineered model to simulate the progressive 3D printing process and predict the generation and progressive effects of void and precipitate on the mechanical properties of engineering alloys. Material properties from a representative steel is used to validate the model. In this model micro-cracks can randomly initiate and grow under a micro-triaxial stress state at positions where accumulated damage reaches critical values. Grain size/distortion and void/precipitate density and distribution simulations are shown as a likely reason for crack branching and growth. The model sets out a novel approach and points the way for analysis of more complex microstructures with different phases and sub-grain particles. The development of such models is likely to be the preferred approach to predict 3D manufactured material properties as well as component failures.

AAAFM-Awards -1: AAAFM-Awards Presentations-1

Time: Thursday, 19/Aug/2021: 8:10am - 10:10am · *Virtual location:* Theatre
Session Chair: Xiangfeng Duan

8:10am - 8:50am

III-Nitride Materials for Full Color Emerging Photonic Applications

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The III-Nitride materials system consisting of the alloys of (Al,Ga,In)N has shown remarkable success in creating new photonic devices. The advent of energy efficient solid-state lighting relied on high quality epitaxial growth of quantum well InGaN/GaN LEDs. Further improvements in III-Nitrides has led to the development of Micro-LED based displays, and GaN based laser for directional illumination. The developments of high performance InGaN based micro-light-emitting diodes (μ LEDs) are discussed. Through novel epitaxial growth and processing, and transparent packaging we have achieved external quantum efficiencies as high as 58% EQE at 450nm. The critical challenges of μ LEDs, namely full-color scheme, decreasing pixel size and mass transfer technique, and their potential solutions are explored. Recently, we have demonstrated efficient microLEDs emitting in the blue to green at dimensions as small of 1 micron. By growing optimized the strain in InGaN nanostructures on porous GaN, we have achieved wavelength as long as 620nm in the III-Nitride materials system. Looking into the future we see GaN Laser Diodes based solid state lighting as impacting high brightness specialty lighting. This work was supported by the Solid State Lighting and Energy Electronics Center(SSLEEC).

8:50am - 9:30am

Water Harvesting from Air Anytime, Anywhere

Omar M. Yaghi

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Water is essential to life. It is estimated that by 2050 nearly half of the world population will live under water stress conditions, due to either arid conditions or lack of access to clean water. This presentation outlines the parameters of this vexing societal problem and presents a potential solution. Since our initial report in 2014 that metal-organic frameworks (MOFs) are capable of trapping water at relative humidity levels as low as 10%, we have shown that they also exhibit facile uptake and release kinetics, and favourable energy requirements. This has led us to carryout field trials in the driest deserts, where kilogram quantities of MOFs were tested in several generations of devices. This presentation will outline results of these field tests and the power of the strong bond, secondary building unit approach in realizing robust MOFs for harvesting water from desert air. We show that the vision of having clean water from air anywhere in the world at any time of the year is potentially realizable with MOFs and so is the idea of giving "water independence" to the citizens of the world.

9:30am - 10:10am

Chemically Tailored 2D Materials for Electronic and Energy Technologies

Mark C. Hersam

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Layered two-dimensional (2D) materials interact primarily via van der Waals bonding, which has created new opportunities for heterostructures that are not constrained by epitaxial growth. However, it is important to acknowledge that van der Waals interactions are not limited to interplanar interactions in 2D materials. In principle, any passivated, dangling bond-free surface interacts with another via non-covalent forces. Consequently, layered 2D materials can be integrated with a diverse range of other materials, including those of different dimensionality, to form van der Waals heterostructures [1]. Furthermore, chemical functionalization provides additional opportunities for tailoring the properties of 2D materials [2] and the degree of coupling across heterointerfaces [3]. In order to efficiently explore the vast phase space for van der Waals heterostructures, our laboratory employs solution-based additive assembly. In particular, constituent nanomaterials (e.g., carbon nanotubes, graphene, transition metal dichalcogenides, black phosphorus, boron nitride, and indium selenide) are isolated in solution, and then deposited into thin films with scalable additive manufacturing methods (e.g., inkjet, gravure, and screen printing) [4]. By achieving high levels of nanomaterial monodispersity and printing fidelity, a variety of electronic and energy applications can be enhanced including photodetectors, optical emitters, supercapacitors, and batteries [5-7]. Furthermore, by integrating multiple nanomaterials into heterostructures, unprecedented device function can be realized including anti-ambipolar transistors, gate-tunable Gaussian heterojunction transistors, and neuromorphic memtransistors [8-10]. In addition to technological implications for electronic and energy technologies, this talk will explore several fundamental issues including band alignment, doping, trap states, and charge/energy transfer across van der Waals heterointerfaces.

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FESC-INV-2: Functional Materials for Energy Storage and Conversion Devices

Time: Thursday, 19/Aug/2021: 8:10am - 10:00am · Virtual location: AU 2410

Session Chair: Elham Sahraei

8:10am - 8:25am

Engineering of low-cost and environmentally benign catalysts for thermal-assisted photocatalytic hydrogen production

Sergey Nikitenko¹, Sara El Hakim², Tony Chave¹

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Conversion of solar energy into hydrogen via photocatalytic splitting of water is an alternative sustainable process of paramount interest for clean energy storage. In this view, preparation of stable and nontoxic catalysts from non-precious elements showing high photocatalytic activity under solar light irradiation is of great importance. Herein, we provide new insights into the design of Ti@TiO₂ core-shell photocatalyst with advanced photothermal activity in the process of hydrogen production from aqueous solutions of glycerol. Ti@TiO₂ nanoparticles have been obtained by sonochemical treatment of titanium metal nanoparticles in pure water. SHT process based on simultaneous hydrothermal and ultrasonic treatment has been proven to be effective for the synthesis of nanocrystalline materials with advanced properties.^{1,2} In general, acoustic cavitation in hydrothermal solutions accelerates the crystallization and improves the catalytic performance of nanocrystalline metal oxides. In this study, we found that variation of SHT temperature allows controlling nanocrystalline TiO₂ anatase shell on TiO surface. At 100<T<150°C formation of TiO₂ nanoparticles occurs mostly by crystallization of Ti(IV) amorphous species and oxidation of titanium suboxide Ti₃O presented at the surface of TiO nanoparticles. At T>150°C, TiO₂ is also formed by oxidation of TiO with overheated water. Kinetic study highlights the importance of TiO₂ nanocrystalline shell for H₂ generation. Electrochemical impedance spectroscopy points out more efficient electron transfer for Ti@TiO₂ nanoparticles in correlation with photocatalytic data. The activation energy (E_a=32±2 kJ·mol⁻¹) assumes that photothermal effect arises from the diffusion of glycerol oxidation intermediates or from water dynamics at the surface of catalyst. Interesting that under the heating photocatalytic H₂ emission is observed even in pure water in the presence of Ti@TiO₂ nanoparticles.

References

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8:25am - 8:40am

Beyond structural and chemical imaging in a TEM -- new opportunities for understanding interfaces in energy materials

Miaofang Chi

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Electron microscopy has enabled imaging and chemical analysis of materials at the single atom level. Substantial contributions to energy materials research have been made in the past decade, especially to the investigation of interfaces, which often act as the bottleneck in next generation energy systems. Many critical interfacial questions remain open and answering them requires us to go beyond the conventional atomic-scale structural and chemical analyses. We must understand the behavior of the electrons and their dynamic evolutions under operation conditions. Recent developments in scanning transmission electron microscopy (STEM), including atomic-scale in situ imaging, four-dimensional (4D)-STEM, and monochromated electron energy loss spectroscopy (EELS) have opened up unprecedented opportunities. In this presentation, I will introduce these capabilities and highlight examples demonstrating how these capabilities allow us to reveal the origin of high interfacial resistance and of the unexpected dendrite growth in all-solid-state batteries, and directly observe anionic electrons in electrides for the first time. Perspectives for the future advancement of these new STEM techniques for research into emerging energy materials will also be provided.

8:40am - 8:55am

Anodized metal oxide nanotubular arrays for gas-phase photocatalysis and photo-induced high-purity hydrogen production

Kei Noda

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So far, in order to enhance photocatalytic activity of metal oxide semiconductor materials with wide bandgaps such as hematite (α-Fe₂O₃) and TiO₂, self-aligned nanotubular structures with large specific surface area prepared by electrochemical anodization have been intensively studied due to their attracting features such as simplicity and low cost fabrication. Electrolytes including both fluoride and polyols for anodic metal oxide have been widely employed owing to their better controllability for obtaining different nanostructures. In fact, well-aligned metal oxide nanotubes with smooth walls were produced and those applications toward water photooxidation and air purification with high performance were demonstrated. In this presentation, I will introduce our recent results on visible-light-responsive gas-phase photocatalysis over the anodized hematite nanotubular arrays loaded with platinum or cuprous oxide (Cu₂O) nanoparticles. In addition, photo-induced high-purity hydrogen production based on a bilayer membrane of an anodized TiO₂ nanotubular array and an electroless-deposited palladium layer will be also presented.

8:55am - 9:10am

Advanced doping techniques for nanostructured solar cells

Rosaria A. Puglisi

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Silicon based solar cells have represented the leading actors in the last decades photovoltaic market share with respect to all the other technologies, thanks to the Si abundance, stability and non-toxicity, and future projections confirm this predominance also in the years to come. However, half of the cell module cost is due to the material used and to its processing. In order to decrease the costs, it is known that a cut in the Si consumption must be operated. This will decrement the optical absorption and consequently the output generated current. To keep the performance level, a large number of special Si surface designs aimed at light harvesting have been proposed. One of the most popular approaches is to use silicon nanowires embedded in the solar cell emitter as optically and electrically active layer. Thanks to their excellent optical properties they have represented the first choice for many academic approaches. In this context conventional doping methods have shown limitations, not yet overcome despite the technological developments, such as use of expensive equipments and materials, need of numerous steps to obtain conformality, formation of structural defects or precipitates and limited control on ultra-shallow diffusion depth. Recently an alternative doping process has been proposed, the molecular monolayer doping (MD) [Nat Mat 7 (2008) 62, Mater Sci Eng B 178 (2013)686, Phys Stat Sol A 212(8) (2015)1685, Mat Sci Semic Proc 42 (2015)200, Appl Mater Interf 8 (2016)4101]. MD provides conformality, does not introduce structural defects, does not use dangerous and expensive sources or equipments and allows to control the junction depth at nanometer level. The process is based on the self-assembling of a molecular monolayer of specific dopant precursors on the Si substrate. Then an annealing step releases the dopant atoms from the monolayer and diffuse them into the substrate. Thanks to the source self-assembling mechanism the dopant atoms density and positions are determined, depending on the molecule steric properties. With MD is possible to achieve junction depths as small as 5 nm and to fabricate FETs and solar cells [Nanoletters 9(2) (2009) 725, Sol En Mat & Sol Cells 132 (2014)118]. The talk will provide a brief overview on the morphological, chemical and physical properties of the assembled molecules, focusing on the characteristics of the molecule/Si interface which plays a strategic role on the electrical performance of the final samples. New results on the dynamics of the molecule modification during the self-assembling and the thermal process, from the chemical and morphological point of view will be also presented. The results of the integration of the molecular doping on silicon nanowires will be shown and discussed, together with the electrical results obtained on the solar cells where the Si nanowires have been integrated as emitters.

9:10am - 9:25am

Laser Scribed Fractal Graphene Capacitors: Scaling Behavior with Respect to Fractal Order and Complexity

Benjamin Barnes¹, Jean Paul Badjo², Christopher Blanks³, Mark Demorra¹, Othman Suleiman³, Kausiksankar Das³

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In past decades, the application of fractals to electrode design for enhanced signaling and electrochemical performance was a popular subject and enabled the growth of consumer micro-electronics. Supercapacitors, which are energy storage devices with many promising characteristics, have largely grown alongside of such developments in electronics, but little work has been done to use fractal electrodes in supercapacitors. In this work, plane-filling and fractal patterns were used in designing laser scribed graphene supercapacitor electrodes, allowing the scaling laws of capacitance with respect to fractal order and complexity to be examined for the first time. An interesting exponential relationship between capacitance and fractal order for the more open structured fractals was observed, the exponent of which was proportional to the Hausdorff dimension. This indicates that two or more competing parameters are at play, likely path resistance and surface area. These results indicate that there is a benefit in using fractal electrodes in supercapacitors, but the magnitude of the benefit depends on the interactions between path length and surface area, and therefore fractal order.

9:25am - 9:40am

Detailed Multiphysics Modeling of a 18650 Cylindrical Lithium-ion Battery

Mohammad Keshavarzi¹, Mehdi Gilaki¹, Youngwon HAHN², Ni SUI², Junwei XING², Victor OANCEA², Elham Sahraei¹

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In this fast-growing electrification era, need for higher energy density and safer batteries to be used in various applications sparks researchers' interests from different fields of study to analyze this multi-physics and multi-scale phenomenon. The layered structure of the lithium-ion batteries includes combination of various components which have different mechanical, electrical and thermal properties. The coupled effects of these physics has made battery modeling a complex problem. Hence, a cost-efficient model to precisely predict the behavior of batteries is in high demand by all the battery related industries. Several publications have investigated the mechanical behavior of batteries in different loading scenarios but a detailed modeling of a battery validated in coupled loading scenarios hasn't been completed. In this study, first a conditioned battery cell was dissected, and samples were prepared from the jellyroll layers. A variety of testing was done on the samples to measure mechanical, electrical and thermal properties of the layers. The structure of the cell components and in-situ jellyroll configurations were extracted using CT-scan of the battery. A model for the cell was developed in ABAQUS Explicit to simulate a combined mechanical electrical loading scenario. The detailed model was validated under combined mechanical/electrical/thermal loading. This comprehensive detailed modeling and the material calibration provide in this study, create a tool for various battery related industries to optimize properties of their products by using battery cell modeling and investigate effects of various component changes or safety features on a fully coupled detailed model. This tool will reduce the timing and costs of the design and development steps to manufacture a safe and high energy/power density product.

9:40am - 9:55am

Organic photovoltaic devices for next generation indoor applications

Wing Chung Tsoi

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Organic photovoltaic devices have attracted significant interest for outdoor energy harvesting, as they have unusual properties including easy tunability of optical and electrical properties, and can be fabricated by low-cost, mass production methods. However, the potential for organic photovoltaic devices for indoor application (i.e. harvesting indoor light for self-sustainable electronics, e.g. power sensors) is much less explored. While there were a few initial studies on this topic, the power conversion efficiency of organic photovoltaic devices under indoor lighting (fluorescence lamp or white LEDs) is still low at that time. In 2016, our team revised the potential of organic photovoltaic devices for indoor applications by using the more state-of-the-art materials (at that time), which demonstrated good efficiency under indoor lighting. By exploring the design rules for indoor light harvesting, in 2018, we demonstrated a record high power conversion efficiency at that time (28% under 1000 lux fluorescent lamp: significantly better than silicon). These two crucial findings have then been leading to very active and significant amount of research on organic photovoltaic devices for indoor applications in the research community. In this talk, I will present the findings (and the design rules, and the perspective), and we believe that organic photovoltaic devices for indoor applications have much more promising potential to be commercialized (compared to outdoor applications), and can have significant impact on powering the "Internet of Things" for smart home, office, supermarket, buildings, etc.

9:55am - 10:10am Warning: This presentation lies outside the session time!

Negative Electrode Materials for Supercapacitive Energy Storage: Bottlenecks and Possible Remedies

Abolhassan Noori¹, Richard B. Kaner², Mir F. Mousavi¹

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Although benefiting from the intrinsic advantages of high-power capability and long cycling stability, the low energy performance has limited, to some extent, broader feasible applications of supercapacitors. 1 Energy of a supercapacitor can be increased by either increasing the device capacitance or extending the operating voltage window. Compared with the positive electrode materials that have made incredible progress thus far, the lack of high capacitance negative electrode materials is still a bottleneck for making further progress toward high device-level capacitance supercapacitors. As a remedy to this challenge, we have pursued some high-capacitance negative electrode materials via grafting organic redox active species onto carbon-based materials. 2,3 In one approach, we conjugated thionine and Nile Blue as redox active aromatic dyes to graphene aerogel via π - π stacking interactions. Via this simple yet effective approach, we obtained highly stable negative electrode materials with enormously higher supercapacitive performances. In another approach, we prepared a CoFe₂O₄-rGO nanocomposite via a scalable one-pot solvothermal method that delivers high capacitance as a negative electrode material. 4 Via these intriguing approaches we have fabricated some high-energy supercapacitor devices without sacrificing their intrinsic high-power capability and long cycling stability.

10:10am - 10:25am Warning: This presentation lies outside the session time!

Merging Nanotechnology & Synthetic Biology toward Directed Evolution of Materials for Photocatalysis

Elena A. Rozhkova

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The light-matter interaction has been making a major impact since the ignition and evolution of life on Earth. It is the cornerstone of modern life-changing technologies, above all, photocatalysis and sustainable energy production. In our work, we use a powerful combination of chemical synthesis, fabrication, and synthetic biology to develop hybrid hierarchical structures from atoms and molecules, resulting in new functions that go far beyond the individual starting components.

This talk will include recent examples of engineered nano-hybrid architectures based on light-gated natural proton pump either isolated from a host microorganism, or produced through cell-free synthetic biology. The fusion of a soft material, including a proton pump, with inorganic nanoparticles, or photonic supra-structures results in a functional "artificial cell" controlled by light. These hybrids demonstrate catalytic activities in H₂ evolution reaction [1-4], CO₂ reduction to value-added chemicals [5], and cell-mimicking synthesis of ATP [6].

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FLNM-INV-2: Fabrication of Low dimensional, Nano and 2D materials

Time: Thursday, 19/Aug/2021: 8:10am - 10:00am · Virtual location: AU 2412

Session Chair: Rainer Timm

8:10am - 8:25am

Colloidal Low-dimensional perovskite: synthetic strategies and optical properties

Raquel E. Galian, Rita Cevallos-Toledo, Ignacio Rosa-Pardo, Julia Pérez-Prieto

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Perovskite materials have emerged as very promising materials for optoelectronic, photovoltaic, and more recently photocatalysis due to their outstanding optical and electronic properties. Lead halide perovskite (LHP) responds to the general formula $APbX_3$, where A is an organic cation such as methylammonium, formamidinium, or inorganic cation such as Cs^+ , and X is a halide anion (Cl^- , Br^- or I^-). LHP can be prepared with different stoichiometries and morphologies: low dimensional material such as 1D nanowires/nanorods, 2D nanosheets/nanoplatelets, and 0D nanoparticles. The first colloidal dispersion of lead bromide perovskite nanoparticles ($CH_3NH_3PbBr_3$) was synthesized using long ammonium salts as organic ligands, resulting in a good luminescence quantum yield (20 %) and stability in a battery of low polar solvents. The preparation of few-layered perovskites with the formula $L_2[APbX_3]_n-1PbX_4$, where L represents the ligands and n corresponds to the number of PbX_6 perovskite layers sandwiched between organic ligands layers have received great attention. They exhibit strong quantum confinement due to their thinness and present very narrow absorption and emission peaks with small Stokes-shift. According to the nature of the organic ligands and the synthetic methodology, we were able to prepare two-layered $[APbBr_3]PbBr_4$ perovskite nanoplatelets with blue-deep emission and good chemical/photochemical stability. Moreover, novel colloidal nanocomposites were obtained in the presence of cycloalkylammonium bromide, lead polymer, and perovskite nanocrystals leading to long, 1D well-defined architectures.

The key role of the organic ligands for surface passivation, the dimension of colloidal perovskite establishment, and the preparation of novel heterostructures together with a general overview of the colloidal perovskite applications will be discussed.

8:25am - 8:40am

Fabrication of Polyethyleneimine conjugated fluorescent MXene nanosheets and its cytotoxic evaluation

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MXene is one of the most exciting 2D materials currently, which has incredible potential in various applications. In this work, we report Polyethyleneimine (PEI) conjugated MXene nanosheets, which are cationic in nature. $PEI_Ti_3C_2Tx$ (PEI_MX) was produced by etching Ti_3AlC_2 , ultrasonicated along with PEI, and then hydrothermally treated at 200 °C for 24 hours. PEI is a positively charged polymer containing repeating amine groups. The as-obtained nanosheets were characterized through XRD, AFM, TEM, UV-vis spectroscopy. The thickness of PEI conjugated nanosheet was found to be 2.63 ± 0.85 nm compared to control 6.82 ± 1.66 nm, proving its utilization both as a surfactant as well as a functionalizing agent. The use of polymer also assists in forming a stable aqueous dispersion. The small-sized nanosheets were found to be highly biocompatible and exhibited blue fluorescence. The photoluminescence of the 2D nanosheets enables them to be also utilized as cell labeling probes. The PEI_MX are highly scalable and their intrinsic NIR activity, fluorescence, small size, and cationic character can be applied for a variety of applications like cell imaging and photothermal therapy.

8:40am - 8:55am

Conjugated Pi-Structures with Different Topologies

Chunyan Chi

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Carbon-based nanostructures have shown revolutionary influence in the areas of chemistry, physics and materials science. Recent efforts have been focused on novel topological structures of sp^2 -carbons such as carbon nanohoops, nanobelts, molecular cages, and open-shell nanographenes, which provoked new chemistry and materials. However, synthesis of this kind of molecules is extremely challenging mainly due to strain or intrinsic high reactivity. Another issue is that most of these carbon nanostructures have a localized aromatic character; that means, the π -electrons are not globally delocalized along the backbone, which limits their optical and electronic properties and applications. Herein, synthesis of a series of novel pi-structures with different topologies will be introduced, and their physical properties, aromaticity and diradical character will be discussed.[1-11] They include: 1) azulene-embedded linear compounds and curved nanographenes; 2) cyclopenta ring fused bisanthene and its charged species with open-shell singlet diradical character and global aromaticity/anti-aromaticity; 3) zigzag-edged nanographene and nanobelts.

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8:55am - 9:10am

Controlling the parity and time-reversal symmetry of graphene Dirac plasmons and its application to terahertz lasers

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Graphene has a unique electronic band structure that is linearly dispersed and gapless. As a result, both electrons and holes behave as relativistic charged particles of massless Dirac fermions. The quantum of plasma oscillation of these Dirac electrons is called the graphene Dirac plasmon, which can dramatically enhance the interaction of terahertz (THz) waves with graphene. We have proposed an original current-injection graphene THz laser transistor, demonstrated single-mode THz laser oscillation at low temperatures¹⁻³, and discovered and demonstrated the THz giant gain enhancement effect by graphene Dirac plasmons^{4,5}). However, in order to realize room temperature high intensity THz lasing and ultrafast modulation operation, which are necessary for the next generation wireless communication of 6G and 7G, further breakthroughs are needed. In this work, we introduce completely new physics and principles to simultaneously break through the limits of quantum efficiency and high-speed modulation operation by actively controlling the parity and time-reversal symmetry⁶) of graphene Dirac plasmons with nanostructures and applied voltages. In this talk, we will present new ideas on the operating principle and device structure of graphene plasmonic laser transistors with high radiation intensity and ultrafast modulation capability operating at room temperature in the THz frequency band.

This work was supported by JSPS KAKENHI #16H06361 and #20K20349, Japan.

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9:10am - 9:25am

Silicon nanowires based artificial neuron

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Learning processes similar to those occurring in a human brain can also be realized relying on brain-inspired computers. To implement a device like a biological neuron, it is necessary to trigger chemical processes occurring in a neuron cell directly within the electronic device. For example, the device should be able to transfer ions or molecules and store their instantaneous distributions as 'states', which should be subsequently controlled in response to external stimuli. Here we report a neurotransistor made from a silicon nanowire transistor coated by an ion-doped sol-gel silicate film that can emulate the intrinsic plasticity of the neuronal membrane. The neurotransistors are manufactured using a conventional complementary metal-oxide-semiconductor process on an 8-inch (200 mm) silicon-on-insulator wafer. Mobile ions allow the film to act as a pseudo-gate that generates memory and allows the neurotransistor to display plasticity. We show that multiple pulsed input signals of the neurotransistor are non-linearly processed by sigmoidal transformation into the output current, which resembles the functioning of a neuronal membrane. The output response is governed by the input signal history, which is stored as ionic states within the silicate film, and thereby provides the neurotransistor with learning capabilities.

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9:25am - 9:40am

Surface functionalization of magnetic nanoparticles for magnetically driven passage through eye tissues for magnetic drug targeting

Silvio Dutz¹, Diana Zahn¹, Katja Klein¹, Patricia Radon², Edgar Nagel^{1,3}, Michael Eichhorn⁴, Frank Wiekhorst²

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If a pharmaceutical agent has to be applied into a patient's eye, for example because of a disease of the retina, a drug administration by an intravitreal injection directly into the vitreous body is a common and very effective strategy. This injection causes severe risks and discomfort for the patient, so that an alternative strategy to target the drug would be very beneficial. Therefore, we are evaluating the possibility of magnetic drug targeting into the eye by using magnetic nanoparticles (MNP) to which the drugs can be linked.

Magnetic nanoparticles with an optimized multicore structure were selected for this application by evaluating the stability against agglomeration of MNP with different functional coatings (e.g. different dextrans, starch, citric acid, PEG) in water for injections, physiological sodium chloride solution, and biological media like artificial tears fluid. From these investigations, starch turned out as the most promising coating material because of its stability in saline fluids due to its steric stabilization mechanism.

To evaluate the passage of MNP through the sclera and cornea of domestic pig (*sus scrofa domestica*) eye tissues, a 3D printed setup consisting of two chambers (reservoir and target chamber) separated by the eye tissue, was developed. With a permanent magnet array, emulating the 20 T/m field gradient of a superconducting targeting setup promising for such targeting as found in simulations, experiments aiming on a magnetically driven transport of the MNP from the reservoir chamber into the target chamber via the tissue were performed. The resulting MNP concentration in the target chamber was determined by means of quantitative magnetic particle spectroscopy (MPS). It was found that, none of the tested particles passed the cornea, but starch coated particles can pass the sclera with a rate of about 5 ng/mm² within 24 hours. These results open the door for a future magnetic drug targeting to the eye.

9:40am - 9:55am Warning: The presentations finish prior to the end of the session!

Defect Engineering in 2D Materials by Non-equilibrium Synthesis and Processing

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Defects in 2D materials significantly impact their structure and properties due to the ultrathin thickness and quantum confinement. In addition, defects in 2D materials can induce phase transitions, stabilize metastable phases, and give rise to the formation of new phases with different stoichiometries. Therefore, it is important to fundamentally understand the defect evolution and precisely control the type, density, and position of defects in 2D materials to tailor their properties and further introduce new functionalities. Here, I will demonstrate the nonequilibrium synthesis strategy to tailor the defect density and type in 2D transition metal dichalcogenides and the emerging properties for optoelectronic and electronic devices. Then I will introduce a defect-mediated phase transition by plasma irradiation in highly anisotropic 2D PdSe₂. With in-situ scanning transmission electron microscopy characterization and theoretical calculations, the defect evolution and defect-mediated phase transformation in PdSe₂ were studied at the atomic scale. Our results showed that depending on the concentration of Se vacancies in PdSe₂, it could change to a variety of palladium selenides with different chalcogen contents. Through selective phase engineering, single material devices based on few-layer PdSe₂ crystal with the new metallic phase as a seamless contact display significantly enhanced electrical performance due to the reduction in contact resistance and Schottky barrier height. Therefore, engineering defects in 2D materials is a promising way to tune their electronic properties and add new functionalities for future applications in optoelectronics and quantum information science.

Research was sponsored by the U.S. Dept. of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Div. and was conducted at CNMS, a U.S. DOE Office of Science User Facility.

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FESC-3: Functional Materials for Energy Storage and Conversion Devices

Time: Thursday, 19/Aug/2021: 10:20am - 12:30pm · Virtual location: AU 2410

Session Chair: Miao Fang Chi

10:20am - 10:30am

The origin of the light-induced phase segregation in mixed halide perovskites

Lyubov A. Frolova¹, Sergey Yu. Luchkin², Ernst Z. Kurmaev^{3,4}, Sergey M. Aldoshin¹, Pavel A. Troshin¹

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Tunability of optoelectronic properties of lead halide perovskites achieved through halide mixing can potentially enable their multiple applications e.g. in tandem solar cells and light-emitting diodes. However, mixed halide perovskites are unstable under illumination due to their segregation into Br-rich and I-rich phases, which negatively affects the performance characteristics and operational stability of devices. Research efforts over the past years provided a substantial understanding of the factors influencing light-induced halide phase segregation. While several mechanisms were proposed, none of them could account for all available experimental data; and hence the origin of the effect is still under active debate. Herein, we thoroughly investigated the photodegradation of CsPbI₂Br and Cs_{1.2}PbI₂Br_{1.2} using a set of complementary techniques. In-situ atomic force microscopy provided a spectacular visualization of the real-time halide phase segregation dynamics demonstrating that iodoplumbate is selectively expelled from the mixed halide perovskite grains and nucleates as a separate I-rich phase at the grain boundaries. We propose a mechanism based on the reversible Pb²⁺/Pb⁰ and I⁻/I³⁻ redox (photo)chemistry, which explains our experimental findings and other previously reported results. Furthermore, it sheds new insights on the underlying mechanisms of multiple phenomena related to light- or electric field-induced degradation of various lead halide perovskites. More details can be found in our recently published paper [1].

Key Words: Perovskite, Phase Segregation, Solar Cells

References

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10:30am - 10:40am

Organic redox-active materials for high-capacity and high-rate potassium-ion batteries

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Using organic redox-active molecules provides a new paradigm for future development of metal-ion batteries. Indeed, organic materials are usually based on light elements (C, H, N, O, S) and, therefore, can enable much higher specific capacities compared to the salts and oxides of heavy transition metals. Most of organic materials are non-toxic and environment friendly, which makes easy their recycling as a common household waste. In contrast to crystalline inorganic cathodes and anodes, organic materials are soft and, therefore, can operate at high charge and discharge rates thus leading to design of ultrafast batteries. Mechanical properties of polymeric cathodes and anodes enable their application in truly bendable batteries for emerging generation of portable electronics.

Lithium-ion batteries currently represent one of the mainstream energy storage technologies. However, lithium is a scarce element and the available resources are definitely not matching the rapidly growing demand for energy storage. Therefore, sodium- and potassium-ion batteries (SIBs and PIBs) are now considered as promising scalable metal-ion battery technologies. In that context, organic redox-active materials are particularly important since they can operate efficiently with multiple mobile ions, while most of inorganic cathodes are constrained to only one specific ion matching the crystal lattice.

In this talk, we will highlight our recent results on the design of organic and metal-organic cathode and anode materials for potassium batteries. In particular, we will present ultrafast potassium-ion batteries delivering specific capacities of 169 mA h g⁻¹ at an impressive current density of 10 A g⁻¹ (charging/discharging in ca. one minute) and 245 mA h g⁻¹ at a lower current density of 50 mA g⁻¹. Specific energy of ~550-600 W h kg⁻¹ is reached for the best organic cathodes in potassium batteries. The polymer-based devices also demonstrated record-high cycling stability with no capacity decay after 4600 cycles, thus outperforming all previously reported non-aqueous K-ion batteries.

The obtained results suggest that organic electrode materials, while being at the infancy of their development, start to show commercially interesting performances thus paving a way to implementation of a new generation of post-lithium metal-ion batteries.

Key Words: Potassium-Ion Batteries, Energy Storage

10:40am - 10:50am

Micro and Nano Structures that Enable 'Bubble-Free' Water Electrolysis that is Highly Energy Efficient

Gerhard F. Swiegers, Aaron Hodges, Linh Hoang, George Tsekouras, Klaudia Wagner, Chong-Yong Lee, Gordon G. Wallace

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Highly efficient electrochemical splitting of water into hydrogen and oxygen constitutes the most critical capability needed for the development of a future hydrogen economy based on renewable energy.¹ In this work we demonstrate that direct conversion of water into hydrogen and oxygen gas, without the intermediacy of gas bubble formation, may notably decrease the energy required. We



report the operation and performance of “bubble-free” alkaline electrolyzers with electrodes that combine catalyst layers containing high-performing water-splitting catalysts, with gas removal structures. The gas removal structures vigorously extract the gases as they are produced by the catalyst layer, before bubbles can be formed. In so doing, the energy penalties arising from bubble formation are avoided. At 80 °C, the best electrolyzer produced ~800 mA/cm² at 95% energy efficiency (1.54 V) and ~400 mA/cm² at 100% energy efficiency (1.47 V), relative to the Higher Heating Value (HHV) of hydrogen. These results constitute an ~20% increase in energy efficiency over present-day commercial alkaline electrolyzers.

10:50am - 11:00am

Exfoliated and Reassembled Graphite Electrodes for Hygroelectricity

Leandra P. Santos¹, Diana Lermen³, André Galembeck², Fernando Galembeck^{1,3}

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Exfoliated and reassembled graphite (ERG) [1] is a new, high-aspect-ratio macroscopic material displaying useful chemical, interfacial, electrical, and thermal properties. Its application to make both electrodes in a hygroelectricity (HE) cell demonstrated the possibility to build large-scale, low-cost devices for distributed, autonomous energy production, including remote environments like humid forests. However, it is necessary to increase HE cells' output by some orders of magnitude to make them useful, which requires a model for their operation. We found a theoretical basis for HE cells in a usually neglected area of classical chemical thermodynamics, that is, electric potential gradients' effect on reaction Gibbs energies within a multiphase system [2]. The chemical effects of electric potential variations are widely explored in electrochemistry but not often in other areas. Most researchers assume the electroneutrality paradigm, notwithstanding the abundant evidence showing the existence of potential gradients in any interface. In the HE cell, the negative electrode owes its charge to adsorbed hydroxide ions while hydronium ions charge the positive electrode. The result is an electrostatic contribution to the reagents' Gibbs energy that increases with the potential difference between the electrodes. The outcome is the less-positive Gibbs energy for the water-splitting reaction that becomes spontaneous when the HE cell voltage reaches 1.63 V. The literature does not yet show HE cells producing such voltages. Still, current results in the >1 V range correspond to equilibrium constants higher than 10¹², thus explaining the continuous delivery of electric current by the HE cells.

A new finding is the positive temperature coefficient of HE cells' power output, implying that the cell operation's reaction is endothermic. Among the candidate reactions that can take place in HE cells, the water-splitting reaction is endothermic, while metal or carbon oxidation reactions are exothermic.

The present results show that the HE cell could also become a source of hydrogen and oxygen released at the electrodes, but it is not as easy as collecting current from the electrodes.

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11:00am - 11:15am

Self-Assembling Monolayers - Effective Approach for Efficient Perovskite Solar Cells

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Perovskite-based photovoltaics promise benefits of low cost, high efficiency and large versatility. However, combining all three factors into one solar cell is a difficult task. In particular, one of the bottlenecks towards large-scale production is the available choice of hole-selective contacts. Self-assembled monolayers as hole-selective contacts are a viable alternative to classic hole transporting materials as they are intrinsically scalable, simple to process, dopant-free and inexpensive. Self-assembly also offers the crucial advantage of conformally covering rough surfaces within a self-limiting, simple to control process, creating energetically well-aligned interface to the perovskite absorber with minimal non-radiative recombination. This approach enables highly efficient single-junction p-i-n perovskite solar cells and record-efficiency monolithic perovskite/CIGSe (24.2%) as well as perovskite/silicon (PCE up to 29.15%) tandem devices.

11:15am - 11:30am

Operando soft x-ray spectroscopy for interfacial characterization of energy-storage materials and chemical transformation

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The energy materials and devices have been largely limited in a framework of thermodynamic and kinetic concepts or atomic and nanoscale. Advanced energy technology arises from the understanding in fundamental science, thus rest in large on in-situ/operando characterization tools for observing the physical and chemical interfacial processes. Synchrotron based x-ray spectroscopic techniques offers unique characterization in many important energy materials of energy conversion, energy storage and catalysis in regards to the functionality, complexity of material architecture, chemistry and interactions among constituents within.

In the operando soft x-ray spectroscopy characterization of interfacial phenomena in energy materials and devices, it has been found that the microstructure and composition of materials as well as the microstructure evolution process have a great influence on performances in a variety of fields, e.g., energy conversion and energy storage materials, chemical and catalytic processes. However, it is challenging to reveal the real mechanism of the chemical processes. In-situ/operando x-ray spectra characterization technique

offers an opportunity to uncover the phase conversion, chemical and environmental change of elements and other very important information of solid/gas and solid/liquid interfaces in real time.

It has been demonstrated how to best use the in-situ/operando soft x-ray spectroscopy characterization techniques, including soft x-ray absorption spectroscopy (XAS) and resonant inelastic soft x-ray scattering (RIXS) to investigate the real electrochemical mechanism during the operation. The experimental results show that in-situ/operando soft x-ray spectra characterization techniques can further enhance the understanding of real reaction mechanism.

11:30am - 11:45am

Structural Origin of Reversible Li Insertion in Guest-Free, Type-II Silicon Clathrates for Applications as Li-ion Battery Anodes

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The guest-free, type-II Si clathrate (Si136) is an open cage polymorph of Si with structural features amenable to electrochemical Li storage. However, the detailed mechanism for reversible Li insertion and migration within the vacant cages of Si136 is not established. Herein, X-ray characterization and density functional theory (DFT) calculations are used to understand the structural origin of electrochemical Li insertion into the type-II clathrate structure. At low Li content, instead of alloying with Si, topotactic Li insertion into the empty cages occurs at ≈ 0.3 V versus Li/Li⁺ with a capacity of ≈ 231 mAh g⁻¹ (corresponding to composition Li₃₂Si₁₃₆). A synchrotron powder X-ray diffraction analysis of electrodes after lithiation shows evidence of Li occupation within the Si₂₀ and Si₂₈ cages and a volume expansion of 0.22%, which is corroborated by DFT calculations. Nudged elastic band calculations suggest a low barrier (0.2 eV) for Li migration through interconnected Si₂₈ cages, whereas there is a higher barrier for Li migration into Si₂₀ cages (2.0 eV). However, if Li is present in a neighboring cage, a cooperative migration pathway with a barrier of 0.65 eV is possible. The results show that the type-II Si clathrate displays unique electrochemical properties for potential applications as Li-ion battery anodes.

11:45am - 12:00pm

Is push-coating the adequate solution to solve the sustainability issue of organic solar cells fabrication?

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Unlike silicon or GaAs based photovoltaics, organic solar cells can be printed at low temperatures and can be manufactured as semi-transparent or flexible devices. Therefore, they receive enormous attention as clean energy source for low-income countries or for energy sustainable cities. However, conventional fabrication of organic semiconductor thin films by spin-coating results in large amounts of hazardous solvent and material being released in the environment (Fig. 1). The work we present here focuses on a thin film fabrication process that considerably reduces the wastes generated during organic solar cell fabrication, which we call push-coating (Fig. 1) [1]. When a silicon elastomer is placed on top of a very small volume of semiconductor solution deposited on a substrate, the solution spreads between the elastomer and the substrate through capillary forces. The solvent then diffuses into the silicon elastomer which results in the formation of uniform semiconductor thin films.

Fig. 1 (included in the attached abstract): Schematic representations of the spin-coating and push-coating processes.

Using push-coating, the amounts of hazardous solvents and material employed can be reduced by 20 and 40, respectively, compared to spin-coating. Additionally, the hazardous solvent can be trapped into the elastomer and easily recycled. We verified that push-coated organic solar cells can yield similar performances to spin-coated ones when using conjugated polymer electron donors and fullerene acceptors [1,2]. However, the results obtained with non-fullerene acceptors are less straightforward and strongly depend on the crystallization dynamics of the semiconductors in the thin films. Nevertheless, our results clearly indicate that push-coating has a great potential for the fabrication of low-cost, green & sustainable organic solar cells.

Key Words: Low-cost, low environmental impact, organic solar cells, sustainable fabrication

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12:00pm - 12:10pm

Developing of Non-graphitizing Carbons as Alternative Materials for Anodes in Li-Ion Batteries

Karolina Jurkiewicz¹, Jakub Kawala², Daniel Szlacheta², Dorota Zygałło¹, Szymon Smykała³, Ewa Talik¹, Paweł Gancarz¹, Joanna Grelska¹, Barbara Liszka¹, Stanisław Duber¹, Andrzej Burian¹

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Carbon anode materials are still under intensive investigation to improve their specific capacity and cycle life in Li-ion batteries [1]. Some non-graphitizing carbon materials prepared by pyrolysis of hydrogen-rich precursors have demonstrated a capacity of more than 1000 mAhg⁻¹, but they have a high irreversible capacity in the first cycle and short cycle life [2]. Therefore, attempts have been made to modify their structure towards better electrochemical properties. We developed glassy carbon and sucrose-based carbon materials modified with various non-carbon additives, which have a catalytic effect on the structural transformation during the graphitization process. The additives are completely removed from the carbon matrix during the heat-treatment at 3000°C. The obtained structures have atypical fiber-like morphology, high degree of graphitization, low surface area and high density, which make them interesting candidates for use as anode materials. By tailoring the type and concentration of the additives, it is possible to

optimize the carbon matrix to deliver the structure with the desired properties. They will be compared with the properties of carbons based on graphitizing coke, commonly used as anode material.

12:10pm - 12:20pm

Ionic Liquids for New Thermoelectrochemical Cells

Veronika Zinovyeva¹, Thomas Salez^{2,3}, Michel Beaughon², Kakoli Bhattacharya², Marco Bonetti², Sawako Nakamae²

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Due to technological progress and population growth, a huge increase in demand for energy is expected in the next years. However, energy production and consumption are accompanied by significant heat losses which generate a direct nuisance on the environment and contribute to climate change. One of the promising routes to new energy resources is the use of this waste heat. In such a context, an interesting way for the direct conversion of low grade heat into electricity is the use of thermogalvanic cells (TGCs) containing ionic liquids (ILs) as electrolyte.^{1,2}

Our choice of the system was focused on the solutions of europium in 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide (EMIM.TFSI). The apparent standard potential of the redox couple Eu(III)/Eu(II) strongly depends on the temperature in various ILs based on the anion TFSI⁻, our objective was therefore to explain this phenomenon and to develop new TGCs.³ We studied the properties of the solutions of europium(III) and (II) as a function of temperature and in the presence of various ligands (water, dimethylsulfoxide, dimethylacetamide, bromides, etc.) by numerous spectral and electrochemical methods.

Cyclic voltammetry study has shown that electroreduction of europium(III) species is irreversible in an anhydrous medium on a glassy carbon electrode. However, the redox process becomes quasi-reversible after the addition of ligands or the temperature increase. In particular, we studied the competitive complexation of europium(III) ions by water and TFSI⁻ or Br⁻ anions over a wide range of temperatures. The diffusion coefficients of the europium(III) species were of the order of 10⁻⁷ cm².s⁻¹ at 61.5 °C. In our work, we have shown that the Seebeck coefficient can reach a record value of -5.5 mV.K⁻¹ due to the competitive complexation of europium ions in ionic liquid medium.

The new TGCs were tested under open and closed circuit conditions, and the obtained data were in perfect agreement with the results of cyclic voltammetry. The electrical power measurements were carried out and the optimization work is underway.

Key Words: Ionic liquids, Europium, Heat Energy Conversion

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12:20pm - 12:35pm Warning: This presentation lies outside the session time!

Touching the forming SEI layer on Li-ion battery anodes

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The successful transition towards electromobility on the ground and in the air alike requires ongoing improvements in the performance of rechargeable battery systems. One bottleneck for state-of-the-art lithium-ion batteries is controlling the so-called solid electrolyte interphase (SEI) which is key for ultimately advancing the life-time of lithium-ion batteries, for obtaining higher rates, and arrive at an increased safety. Interfaces are essential in electrochemical processes, providing a critical nanoscopic design feature for composite electrodes used in Li-ion batteries. Understanding the structure, wetting and mobility at nano-confined interfaces is important for improving the efficiency and lifetime of electrochemical devices. For Si and Si-composite materials used as anodes the interfaces still pose a major issue. Employing additives and using for characterization an electrochemical surface force apparatus, atomic force microscopy, and (hard) X-ray photoelectron spectroscopy it is possible to control the growth and to investigate the mechanical properties of an SEI in a lithium-ion battery

environment. With a new approach of an electrochemical "battery" SFA we present first studies on a gold model system^{1,2} and graphene³ anodes. The force behavior reveals a compressible film at all stages of SEI growth³ and can be used to study wetting phenomena² in confined geometries. The demonstrated methodology provides a unique tool for analyzing electrochemical battery interfaces, in particular in view of alternative electrolyte formulations and artificial interfaces.

References

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FLNM-2: Fabrication of Low dimensional, Nano and 2D materials

Time: Thursday, 19/Aug/2021: 10:20am - 12:30pm · Virtual location: AU 2412

Session Chair: Gerd Grau

10:20am - 10:30am

Molecular Interactions Between Ti₃C₂ MXene and Amine Containing Molecules in Aqueous Buffered Solutions

Swapnil B. Ambade¹, Laura A. Kesner¹, Alicia M. Tripp², Priyanshu Banerjee³, Deepa Madan³, Robert J. Hamers², Zeev Rosenzweig¹

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MXenes, a family of ultrathin layered two-dimensional (2D) transition metal carbides, nitrides, and carbonitrides are steadily advancing as novel inorganic nanosystems for various electronic applications. While the metallic conductivity, solution processability, hydrophilic nature, and presence of various surface functional groups enable the use of 2D MXenes in aqueous systems possible, studies aiming to use MXenes in aqueous and especially biological systems are limited. We investigated the structural and functional properties of Ti₃C₂T_x (T = F, OH) MXenes in N-substituted biological buffers like N-(2-Hydroxyethyl)-piperazine-N'-ethanesulfonic acid (HEPES) and 3-(N-morpholino)-propane sulfonic acid (MOPS) and with a series of amine-containing small molecules when dissolved in phosphate buffer solution. UV-Vis measurements of MXenes when dissolved in solution reveal a striking impact on their absorption spectra in the presence of amine-containing molecules. XRD and electrical conductivity measurements of MXene films which were exposed to amine containing molecules clearly show that these molecules intercalate between MXene nanosheets and significantly affect their electrical conductivity. The interactions of Ti₃C₂T_x MXenes with amine-containing molecules is structure-dependent and are fully reversible. This suggests the interactions are driven by weak bonding interactions like hydrogen bonding and/or electrostatic interactions. This study is an important step toward understanding the stability of MXenes in aqueous media, and the ability to predict the interactions of MXenes and small amine-containing molecules and later larger biomolecules. The reversible nature of the interactions between MXenes and small amine-containing molecules, revealed in our study, open new possibilities for the development of MXenes containing chemical sensing thin films for use in aqueous media.

10:30am - 10:40am

2D Perovskites for Color-Tunable Light Emission

Balaji Dhanabalan¹, Giulia Biffi¹, Seda Kutkan¹, Miao-Ling Lin², Yu-Chen Leng², Ping-Heng Tan², Milena Arciniegas¹, Roman Krahne¹

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Two-dimensional metal halide perovskites are novel materials that have attracted great interest for the development of next-generation optoelectronic devices due to their outstanding figures of merit in photovoltaic solar cells, and in light-emitting devices, which come along with high defect tolerance, low-cost solution processing and tunable emission across the visible spectrum. They consist of atomically this alternating organic and inorganic layers, and this highly anisotropic architecture provides unique elastic, dielectric, and optoelectronic properties that lead to peculiar phenomena, such as self-trapping of excitons due to local lattice distortions. Furthermore, the strong confinement of the charge carriers in the inorganic layers makes such structures natural quantum wells that are appealing for fundamental research and photonic applications. Recently, our group demonstrated how the choice of the type of organic molecules can be exploited to engineer the optical properties of these 2D materials.¹⁻⁴ Here we deepen this approach by a systematic study of their photophysics and vibrational properties at room and cryogenic temperature. The self-trapped exciton emission strongly depends on the organic cation type and temperature. Similarly, the rich spectrum of vibrational resonances is governed by the organics that determine the distortions of the single octahedra layers.

10:40am - 10:50am

Fabricating Three Dimensional Self-Aligning Nanoparticle-based Structures as Gas Sensor Array

Nishchay A. Isaac, Leslie Schlag, Johannes Reiprich, Pedro H. O. Moreira, Alper K. Soydan, Joerg Pezoldt, Heiko O. Jacobs

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Three-dimensional (3D) nanoparticulate bridge structures are demonstrated as room temperature operated, low power gas sensors in this study. 3D morphologies have potential to overcome technological/economic challenges faced in 2D planar homogenous film applications. Fabricated using gas phase electrodeposition, this concept can guide charged nanoparticles to predetermined locations on a surface with sub micrometer resolution. Sequential shutter free deposition is possible, preventing use of additional steps for lift-off and improving material yield. The developed device - a room temperature operated sensor chip; can integrate an array of different nanostructured materials arranged in a pre-decided pattern on the substrate. Each gas sensitive structure is a 3D nanobridge, composed of porous but electrically conducting nanoparticle network. Method of gas phase electrodeposition has been reported [1] and used as interconnects in nanoelectronics. Extending the basic principles for self-aligned growth of nanobridges with a new substrate design, it is possible to grow bridges of different materials on a single substrate to accomplish a single chip "electronic nose" like sensor array with orthogonal sensing capabilities and multi gas sensitivity and selectivity. From an experimental point of view, the method uses a spark discharge-based nanoparticle source in combination with sequentially biased surface electrodes and charged photoresist (dielectric) patterns to accomplish electrodeposition. In total, 1080 Platinum, Nickel oxide and Gold nanobridges are grown to detect Ammonia, Carbon Monoxide and Hydrogen Sulfide gases, respectively. Response and recovery times for these sensors at three different target gas concentrations are reported. The as-deposited bridges have a sensor drift, which can be decreased by 80%



with a stabilization cycle of exposure and removal of target gas. The final gas sensor can detect target gases within minutes and have low sensor signal drift. Additionally, this study highlights the challenges that need to be systematically studied to realize the full potential of programmable approach towards gas phase electrodeposition.

References

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10:50am - 11:00am

Experimental demonstration of absorption enhancement of single layer graphene in optical resonant cavities

Abedin Nematpour, Nicola Lisi, Laura Lancellotti, Rosa Chierchia, Maria Luisa Grilli

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Electric field enhancement at the center of a Fabry-Perot cavity was exploited for enhancing the absorption of single layer graphene. Large area single layer graphene grown by chemical vapor deposition was embedded in different optical resonant Fabry-Perot cavities with central wavelengths in the Vis, NIR and IR spectral ranges.

Fabry-Perot filters were fabricated by radio frequency sputtering starting from alternate quarter wave thickness layers of a high refractive index (H) and a low refractive index material. Film materials and substrates were chosen according to the selected spectral ranges. A thin MgF₂ layer was evaporated onto graphene layers prior to sputtering process to reduce the sputtering induced damage of graphene.

Experimental absorption values were found in very good agreement with those modeled with COMSOL Multiphysics software.

11:00am - 11:15am

Role of carbon Materials in Hydrogen Gas Sensing Application

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The development of gas sensors for the detection of toxic gases like NH₃, CO and H₂ existing in the atmosphere. Among these gases, H₂ is odorless, colorless and flammable at concentrations greater than 4%. However, H₂ is explosive over the range of 15% at standard atmospheric temperature. H₂ gas is predictable to be extensively used as an energy source for fuel cells and it has wide applications in civil transportation. Therefore, H₂ gas sensor is necessary to ensure safe operation of hydrogen based energy storage systems and facilities such as H₂ gas stations, fuel cell based vehicles, semiconductor manufacturing and in rockets for space vehicles, since H₂ leakage leads to explosive accidents. To shun this accidents, H₂ gas sensors have been developed using carbon nanotubes (CNTs), Graphene, Carbon nanomaterials, carbon horn and their nanostructures with metal/metal oxides nano-particles. However, in the present work, the inexpensive candle carbon soot (CCS) is used to detect 0.5% concentration of H₂ gas at room temperature. A simple flame of candle is used to synthesize the layers of carbon soot at room temperature conditions. It is observed that, the acid treatment of CCS drastically improved their structural and sensing properties as compared to as-synthesized CCS. The effect of acid functionalization on the CCS structure were investigated by X-ray diffraction (XRD) and Raman spectroscopy. To the best of our knowledge, detection of low concentrations of H₂ gas is reported here for the first time using economical CCS at room temperature. These results are important for developing a new class of chemiresistive type gas sensor based on change in the electronic properties of the CCS.

11:15am - 11:30am Warning: The presentations finish prior to the end of the session!

Forming input/output (I/O) interfaces with excitable cells and tissue using nanocarbons

Tzahi Cohen-Karni

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We focus on developing a new class of nanoscale materials and novel strategies for the investigation of biological entities at multiple length scales, from the molecular level to complex cellular networks. Our highly flexible bottom-up nanomaterials synthesis capabilities allow us to form unique hybrid-nanomaterials that can be used in various input/output bioelectrical interfaces. For example, we have developed several bioelectrical platforms based on graphene, a two-dimensional (2D) atomically thin carbon allotrope. We have demonstrated recording of the electrical activity of excitable cells with graphene-based ultra-microelectrodes as small as the size as an axon ca. 2µm in size. Using graphene-based hybrid-nanomaterials, we have formed remote, non-genetic bioelectrical interfaces with excitable cells and modulated cellular and network activity with high precision and low needed power. We have also developed a breakthrough bioelectrical interface, a 3D self-rolled biosensor arrays (3D-SR-BAs) of either active field effect transistors or passive microelectrodes to measure both cardiac and neural spheroids electrophysiology in 3D. Our approach enables electrophysiological investigation and monitoring of the complex signal transduction in 3D cellular assemblies toward an organ-on-an-electronic-chip (organ-on-e-chip) platform for tissue maturation investigations and development of drugs for disease treatment. In summary, the exceptional synthetic control and flexible assembly of nanomaterials provide powerful tools for fundamental studies and applications in life science and open up the potential to seamlessly merge either nanomaterials-based platforms or unique nanosensor geometries and topologies with cells, fusing nonliving and living systems together.

AAAFM-Awards -2: AAAFM-Awards Presentations-2

Time: Thursday, 19/Aug/2021: 10:30am - 12:30pm · Virtual location: Theatre

Session Chair: Paul S. Weiss

10:30am - 11:10am

Smart and Programmable Sponges for protection From Bench to Market

Omar K. Farha

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Abstract: MOFs are a class of porous, crystalline materials composed of metal-based nodes and organic ligands that self-assemble into multi-dimensional lattices. In contrast to conventional porous materials such as zeolites and activated carbon, an abundantly diverse set of molecular building blocks allows for the realization of MOFs with a broad range of properties. We have developed an extensive understanding of how the physical architecture and chemical properties of MOFs affect material performance in applications such as catalytic activity for chemical warfare agent detoxification. This talk will focus on metal-organic frameworks (MOFs) for hydrolysis from solution-phase to solid-state reactivity. Moving MOFs from bench to market within industrial sectors will be discussed as well.

11:10am - 11:50am

Tailoring Nanoscale Light with Polaritonic Metasurfaces

Andrea Alù

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Polaritons are formed by material resonances strongly coupled with light. In this talk, I discuss our recent efforts in the context of nano-optics and photonics, with a special emphasis on strong light-matter interactions enabled by exciton, phonon and electronic resonances in polaritonic metasurfaces. I will discuss our recent theoretical and experimental results in the context of hyperbolic polariton manipulation, valley exciton control, twisted bilayers for polariton canalization and extreme dispersion engineering, and giant optical nonlinearities arising in polaritonic metasurfaces based on transition metal dichalcogenides and oxides, boron nitride, graphene and multiple quantum wells. During the talk, we will discuss the exotic light-matter interactions arising by strongly coupling material and optical resonances, stemming from the combination of material and nanophotonic engineering, and the various opportunities that these systems enable for wave physics and photonics technology.

11:50am - 12:30pm

Skin-inspired organic electronics

Zhenan Bao

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Skin is the body's largest organ, and is responsible for the transduction of a vast amount of information. This conformable, stretchable, self-healable and biodegradable material simultaneously collects signals from external stimuli that translate into information such as pressure, pain, and temperature. The development of electronic materials, inspired by the complexity of this organ is a tremendous, unrealized materials challenge. However, the advent of organic-based electronic materials may offer a potential solution to this longstanding problem. Understanding of the materials design enabled arrangement of new applications in medical devices, robotics and wearable electronics. In this talk, I will describe our recent progress in developing chemistry for photo-patterning to enable large scale and high-density fabrication of skin-inspired electronic circuits. I will discuss genetically-targeted chemical assembly as a new way to interface electronics with biological systems in a cell-type specific way.

EPMM-3: Electronic, Photonic and Magnetic Materials

Time: Thursday, 19/Aug/2021: 1:00pm - 3:00pm · Virtual location: AU 2410

Session Chair: Lei Fang

1:00pm - 1:15pm

Applying Computational Materials Science to Crystalline and Nano-Crystalline Magnetic Materials Design

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COVID-19 pandemic is changing our social infrastructure faster than we realize and rapidly revolutionizing the transportation sector industry. The significantly changing sector we face is the goods delivery system in urban and suburban areas. The delivery system uses small gasoline trucks and electric drones for now and will eventually change them to autonomous, medium-powered electric trucks and drones with high-speed data transfer communication system such as 5G; and even 6G networks. Motor quality and cost primarily determine the electric truck and drone's performance and economy. The critical component and most expensive part of a truck or drone's motor are magnetic materials. Therefore, one needs to develop a rare-earth (RE) free, permanent magnet with high maximum energy product (BH)_{max} and also nano-crystalline soft magnet with high magnetization, high electrical resistivity, and small magnetostriction. Computational materials science has a crucial role in the discovery or advancement of magnetic materials.

We will introduce computational materials design methods and present our recently studied RE-free permanent and nano-crystalline (amorphous) soft magnets. Future research work on magnetic materials will be suggested.

1:15pm - 1:30pm

CAN MAGLEV TRANSPORTATION BECOME ONE OF THE MAIN APPLICATIONS OF SUPERCONDUCTORS ?

PIERRE BERNSTEIN, JACQUES NOUEM, YITENG XING

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Magnetically levitated (MAGLEV) transportation systems are more and more considered as alternatives to classical railways. In this contribution, we'll detail the different technologies [Electro-Magnetic Levitation (EML), Electro-Dynamic Levitation (EDL) and Superconducting Magnetic Levitation (SML)] explored and the present realizations emphasizing their advantages and disadvantages. Then, we'll focus on Superconducting Magnetic Levitation. We'll detail the properties of the magnetic field sources and of the superconductors employed and the magnet-superconductor interaction. We'll describe the main numerical simulation techniques and analytical calculations used to reproduce the behavior of levitating systems. Finally, we'll report recent results obtained by our group on the conditions of stability of levitating systems and for increasing their levitation force.

1:30pm - 1:45pm

Computational Design and Optimization of Future Plasmonic Materials and Nanostructures

Jost Adam

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Working with plasmonic and electronic materials involves many scientific steps, including, aside from the laboratory-level experiments, the numerical creation, their comparison, and the device fabrication. Besides these challenging steps, the design of new plasmonic materials with unique physical and chemical characteristics, and outstanding optical properties, which are traditional realms of gold and silver, merits an important place. Optimizing the material properties to improve their functionality and performance in plasmonic applications is a subsequent challenge to be tackled, also through iterative feedback from the experiments. This presentation will demonstrate an overview of recent advances in the computational design of potential future plasmonic materials, such as translational metals, transparent conducting oxides, or plasmonically active semiconductor allotropes, and their application in plasmonic structures, concepts, and devices. The extraction of complex dispersion characteristics from density functional theory (DFT) calculations allows the integration into subsequent electromagnetic modeling steps. We specifically demonstrate the search for new alternative plasmonic materials by manipulating the characteristic response of material candidates such as Al/Ga doped Zinc Oxide (A/GZO), ZrN, TiN and Silicon allotropes. We first perform a series of DFT calculations, including the structural relaxation of plasmonic material candidates, to find the crystal structure with minimum energy, for different exchange-correlation functionals such as GGA, LDA. Secondly, we analyse the simulated material's electronic and optical properties to illustrate potential metallic behaviour, via the electronic density of states (DOS) and subsequently extracted optical dispersion parameters, such as complex refractive index data, Drude-Lorentz parameters, and complex dielectric permittivity. These dispersion data can finally be fed into any electromagnetic simulation tool appropriate to any desired optical system, to investigate its efficiency for suitability in plasmonic applications. Our method comprises the possibility for verification with experimental data on each level. It further admits optimizing digitally the molecular structure, paving the way to predict the proposed compounds' plasmonic functionality, overcoming the persistent hurdles introduced by pure experimental works. We will further introduce the recently developed "Photonic Materials Cloud," a cloud-based platform to support streamline the experimental, numerical, research, and education-based work on plasmonic materials. It allows for creating and comparing various material data via various methods and applying them to standard photonic or plasmonic applications, such as nanoparticle scattering and layered thin-film responses. The export of publication-ready graphics and column-based data facilitates its easy integration into a photonic materials science research line.

1:45pm - 2:00pm

Highly mismatched alloys as a new platform for mid-IR plasmonics

Hassan Allami, Jacob J Krich

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Highly mismatched alloys (HMAs) are semiconductors with strongly modified band structures due to the alloying of elements with strongly different electronegativities. Their band structures have been well described using the band anticrossing (BAC) model,¹ according to which the alloy interaction splits the conduction or valence bands. In the case of a conduction band (CB) anticrossing, the CB splits into an upper (E+) and lower (E-) band, with a rapid change in the band gap as the alloy concentration changes. This large tunability has been used in LEDs and multijunction solar cells. We present these materials as plasmonic resources. We describe the unique plasmonic properties of HMAs with conduction band anticrossings when the E- band is occupied, either by doping or photoexcitation- Using a disorder-averaged Green's function method, which goes beyond the BAC and approximately accounts for the alloy disorder, we determine the bulk plasmon frequency² and the E- to E+ absorption spectrum. We show the distinctive signatures of the direct and indirect absorption processes, which are different from those in standard semiconductors. We further describe a nonstandard scaling of the plasmon frequency, which does not reduce to the free-electron-gas form even when doping is low and the band is well approximated as parabolic. The proven tunability of HMA band structures permits a wide variety of plasmon frequencies to be realized, with the most commonly considered HMAs having resonances in the mid-IR. This exploration helps open up this new material class for plasmonic development.

References

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2:00pm - 2:15pm

Recent Advances in Donor-Acceptor Type of Intrinsically Conducting and Infrared Emitting Polymers

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Impressed by the metallic conduction and superconducting behavior of poly(sulfur nitrile), also called, polythiazyl, discovered by F.P. Butt, in 1910, Alan Heeger, Alan McDiarmid and Hideki Shirakawa, worked on improving conductivity of unprecedently prepared polyacetylene by exposing to iodine vapor in late 70's. These materials have extended conjugation in their polymer backbone that acts as electronic conduction path and charge carriers such as solitons, polarons and bipolarons to conduct electricity. The traditional electronically conducting polymers are (i) carbon-based ones such as polyacetylene, poly(para-phenylenevinylene), poly(azulene), heteroatomic aromatic compounds such as polypyrrole, polythiophene, polyfuran, polyaniline, their derivatives, to name a few. Most of them do not possess intrinsic electrical conduction but the conductivity could be improved by several orders of magnitude by either p- or n-doping. Although, these polymers have a wide range of applications, their processability is very poor owing to their insolubility in common solvents, brittleness and poor mechanical properties. Some of these problems have been addressed by attaching side-chains such as long alkyl chains and alkylenedioxy groups (PEDOT) and so on. The third generation of electronically conducting polymers are the so-called donor-acceptor- (D-A) type polymers, also called push-pull polymers, where the polymer backbone consists of conjugated moieties of donor and acceptor molecules as monomer units. The commonly used donors are electron rich monomers such as thiophene, bithiophene, terthiophene, benzodithiophene, indacenodithiophene, cyclopentadithiophene and common acceptors are diketopyrrolopyrrole, thienopyrrolo-dione, benzothiadiazole, 5,6-difluoro benzothiadiazole, where the acceptors are electron deficient aromatic molecules containing strongly electron-withdrawing groups. These polymers have very low band gaps capable of absorbing and emitting in the visible, near infrared and mid-infrared regions and intrinsic electronic conductivity. Functional D-A type polymers can be developed by backbone engineering and side-chain engineering. Their properties can be optimized by carefully selecting D moieties with low LUMO levels and A moieties with high HOMO levels. D-A polymers with TFT mobilities nearing or surpassing 1 cm² V⁻¹ s⁻¹. The polymers have a myriad of applications in organic thin film transistors, organic photovoltaics (bulk heterojunction devices), bioelectronics, and as supercapacitors.

2:15pm - 2:30pm

Room-temperature ferromagnetism in 2D vdW Fe₃GeTe₂ and its potential application

Tianxiao Nie

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Since the discovery of single-layer graphene in 2004, two-dimensional (2D) van der Waals (vdW) materials represented by it have demonstrated excellent electrical, magnetic, mechanical and optical physical properties under the structure of one or several layers of atomic thickness. Based on these superior properties, 2D-layered vdW ferromagnetic materials have become the basis for constructing low-dimensional spintronics devices, in which Fe₃GeTe₂ (FGT), Cr₂Ge₂Te₆ and CrI₃ as the main representative materials exhibit strong perpendicular magnetic anisotropy and other important characteristics in single layer. However, the Curie temperature (T_c) of above materials has not reached room temperature yet, which has greatly hindered the subsequent development for device application. Therefore, recently researchers have been committed to explore 2D vdW ferromagnetic materials for room-temperature T_c in both theory and experiment. Here, we report that the interfacial engineering effect could effectively increase the T_c of the 2D vdW ferromagnetic material FGT from 230 K to 400 K, through heteroepitaxy with topological insulator of Bi₂Te₃. A theoretical calculation was further carried out to describe the magnetic properties by using first-principles calculations and the self-consistent Hubbard U approach (DFT+Uscf) together with the Monte Carlo (MC) simulations. After combination with Bi₂Te₃, the intralayer interactions in FGT was calculated to dramatically increase compared to that in pure FGT, well explaining the T_c enhancement. Furthermore, we realize the high-efficiency SOT switching of Bi₂Te₃(8)|FGT(4) at room temperature with a write current density of 2.2x10⁶ A/cm² through electrical transports. The experimental analysis of harmonic voltage measurements displays

that the topological surface state of Bi₂Te₃ at room temperature has achieved the magnetization switching of FGT as the main contribution. In particular, the thermal effect in the heterostructure can be reduced by varying the thickness of FGT, which originates from the large anomalous Nernst effect of FGT. Moreover, we report the oxidation process of FGT films exposed to the atmospheric air, which was studied by X-ray photoelectron spectroscopy measurements. The conclusion provides information for the subsequent growth and protection of FGT films, which facilitates the in-depth study of other properties. Our results may open up a new door to benefit the magnetic order in the 2D limit and realize spintronic devices based on 2D-layered vdW ferromagnetic materials with room temperature performances towards industrialization.

2:30pm - 2:45pm

Semiconductor Diamond Electronics and MEMS sensors

Meiyong Liao

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Diamond with an ultra-wide bandgap 5.5 eV shows potential performance that is extraordinarily superior to those of the currently available wide-bandgap semiconductors for energy-saving electronic and microelectromechanical systems (MEMS) devices. For example, the ultra-wide bandgap of diamond enables a high blocking voltage switching devices, and the low mechanical loss offers mechanical resonators with ultra-high quality (Q) factors for sensing applications. For power devices, from the viewpoint of low energy loss, safety aspects, gate reliability, and electronic circuit simplicity, normally-off field-effect transistors (FETs) with low subthreshold slope (SS) values and tunable threshold voltages are strongly in demand. Junction FET by using p-n junction or Schottky metal gate is the traditional method to achieve normally-off operation. Nevertheless, n-type dopants with shallow energy levels in diamond is notoriously difficult. While for metal-semiconductor FETs (MESFETs), there is an intrinsic problem of forward bias limitation.

Here, we propose and demonstrate a device concept of metal-insulator-metal-semiconductor FET (MIMS-FET) based on p-type diamond surface channel to overcome the drawbacks of MOSFET and MESFET. On the other hand, we developed single crystal diamond (SCD)-on-SCD MEMS resonators with ultra-high Q factors over 1 million by using a smart-cut method. We describe a robust and high-performance on-chip SCD NEMS/MEMS by proposing a transduction scheme called self-sensing enhancing actuation (SEA) with integrated actuation and sensing. Diamond MEMS magnetic sensor is also reported in this talk.

2:45pm - 3:00pm

Strain engineering of epitaxial oxide heterostructures beyond substrate limitations

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The limitation of commercial single-crystal substrates and the lack of continuous strain tunability preclude the ability to take full advantage of strain engineering for further exploring novel properties and exhaustively studying fundamental physics in complex oxides. Here we report an approach for imposing continuously tunable epitaxial strain in oxide heterostructures beyond substrate limitations by inserting an interface layer through tailoring its gradual strain relaxation. Taking BiFeO₃ as a model system, we demonstrate the introduction of an ultrathin interface layer allows the creation of desired strain states that can induce phase transition and stabilize a super-tetragonal phase as well as morphotropic phase boundaries overcoming substrate limitations. Continuously tunable strain from tension to compression can be generated by precisely adjusting the interface layer thickness, enabling the achievement of continuous O-R-T phase transition. This proposed route could be extended to other oxide heterostructures, providing a platform for creating exotic phases and emergent phenomena.

FCM-3: Functional Composite Materials

Time: Thursday, 19/Aug/2021: 1:00pm - 3:00pm · Virtual location: AU 2412

Session Chair: Swapnil B. Ambade

1:00pm - 1:15pm

Smart Carbon Fiber Composite Structures Utilizing Printed Electronics

Gerd Grau, Jiefeng Qiu, Mohamad K. Idris

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Carbon fiber reinforced polymer (CFRP) composites are becoming increasingly common for applications such as aerospace, automotive or construction due to their superior mechanical properties. However, one challenge is predicting the failure of CFRP structures under real-world operating conditions due to the complex structure of woven or braided carbon fibers embedded in a polymer resin. This can be overcome by in-situ monitoring of the strain and damage state of CFRP structures. The carbon fibers themselves can be used for this purpose since they are electrically conductive. However, woven carbon fibers in CFRP act essentially as a uniform 2D conductor, which has limited uses for measurements that require location specificity. In order to create smart CFRP structures, the carbon fibers need to be integrated with other electrically functional materials that are patterned to achieve location specificity or other desired functionality. To do so with traditional electronics manufacturing technology is difficult and expensive. Conversely, printed electronics is well suited to this application as it is inherently compatible with fabricating large-area electronic systems on non-traditional substrates.

In this talk, we will discuss our recent progress creating smart CFRP structures by printed electronics. We will show a process of printing electrodes directly onto woven carbon fibers that are subsequently infused with epoxy resin to create 3D CFRP structures. One application of these contacts is to create self-heating CFRP for aircraft de-icing. We will also show how CFRP damage can be detected using printed contacts whose location has been carefully designed together with the measurement protocol and data read-out circuit to achieve location specificity. More complex multi-layer devices can also be fabricated on CFRP structures. We have fabricated electroluminescent devices where the electrodes are a structural carbon fiber weave and a transparent carbon fiber veil. This can be used to light up CFRP structures as well as visually detect the location of strain and damage. These proof-of-concept demonstrations showcase the power of integrating CFRP with printed electronics to create many other forms of smart CFRP structures in the future.

1:15pm - 1:25pm

Fracture Mechanics of Phase-Separated Glasses by Peridynamics Simulations

Longwen TANG¹, N. M. Anoop Krishnan², Jonathan Berjikian¹, Jared Rivera¹, Morten M Smedskjaer³, John C. Mauro⁴, Wei Zhou⁵, Mathieu Bauchy¹

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Although oxide glasses have many unique properties, their range of applications remains limited by their brittleness. By mimicking the microstructure of composite materials, the presence of controlled nanoscale phase separation in glass could overcome this limitation. However, the nature of the toughening mechanism induced by such nanostructuring remains poorly understood. Here, based on peridynamic simulations, we investigate the effect of nanoscale phase separation on the crack propagation mechanism. We show that phase separation can significantly increase glass's toughness (with up to a 90% increase in the fracture energy for the range of conditions investigated herein). The extent of toughening is found to arise from a balance between the overall cohesion of the phase-separated glass and the propensity for crack deflection. This suggests that controlled nanoscale phase separation is a promising route toward the development of tough, yet optically transparent glasses.

1:25pm - 1:35pm

Sandwich-structured composite materials for WiFi antenna application

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In recent years, structurally integrated antennas are growing of interest as the attachment of conventional antennas at the surface of composite material panels impacts their structural integrity [1, 2]. In this study, we investigate a sandwich-structured composite panel made of a honeycomb, E-glass fiber and carbon-fiber pre-impregnated tissues with epoxy resin (prepreg) for WiFi antenna application at 2.45 GHz.

The radiating element is a 35 mm × 35 mm square 370 μm-thick carbon-fiber tissue exhibiting a sheet resistance value $R_s = 0.15 \Omega/\text{sq}$. This carbon element is embedded into a sandwich-structured composite material made of E-glass fiber and epoxy resin prepreg tissues (exhibiting dielectric permittivity $\epsilon_r = 5.0$ and loss tangent $\tan\delta = 0.01$ at 1 GHz) and honeycomb ($\epsilon_r = 1.1$ and $\tan\delta < 10^{-4}$ at 1 GHz). The carbon radiating element is fed by a carbon microstrip line through a coupled slot in the carbon ground plane (Fig. 1). A reference antenna using plain copper sheets (68 μm-thick and $R_s = 2.5 \times 10^{-4} \Omega/\text{sq}$) for the radiating element, the feeding line and the ground plane has also been fabricated with the same size.

The pattern of both antennas has been designed to operate at 2.45 GHz using a 3-D commercial electromagnetic software. Microwave performance of the carbon sandwich-structured composite antenna has been compared with that of the metal counterpart up to 3 GHz. Measurements of the input impedance, radiation pattern and gain demonstrate the relevance of the carbon-fiber tissues to fabricate a pure sandwich-structured composite antenna for wireless application.

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1:35pm - 1:45pm

Engineering nanomaterials based multi-functional interfaces for cytokine biosensing: from nanosensors to in vivo medical devices

Shengnan Ni¹, Zhuping Shen¹, Jagjit Kaur², Laicong Qiao², Chaomin Cao¹, Guozhen Liu^{1,2}

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Cytokines, low molecular weight (~6-70 kDa) soluble proteins secreted from the immune and non-immune cells are core indicators of the functional status of the body. Consequently, monitoring cytokine secretions has enormous value in biology and medicine. Unfortunately, probing cell secretions as they respond in real time to the surrounding signals is still a major challenge as the processes tend to be transient and small molecular size of cytokines, combined with low concentration (in the pM range) and possible interferences in matrix samples. The traditional method for cytokine detection relies on ELISA, which however is expensive, time consuming and incapable to realize real-time monitoring.

By integrating with nanotechnology, biosensors as the analytical devices for the detection of an analyte, that combines a biological component with a physicochemical detector, have demonstrated huge potential for cytokine sensing. Functional nanomaterials possess good conductivity, catalytic activity, biocompatibility and high surface area. This presentation will highlight our recent studies on engineering the sensing interface with functional nanomaterials to achieve novel biosensors for detection of cytokines with improved performances in terms of sensitivity, selectivity, stability and simplicity. These nanomaterials powered sensing platforms include nanosandwich assays, nanosensors, and graphene oxides based and aptasensors, which can be applied for cytokine detection from point-of-care diagnostics to in vivo real-time monitoring. The strategies for fabrication of non-fouling biosensing interface will be discussed. Finally, strategies for fabrication of hydrogel based biosensing devices such as sweat wearables and implantable chips, for continuous cytokine monitoring, will be presented.

Key Words: Nanomaterials, Biosensors, Cytokines, Surface modification, Medical devices

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1:45pm - 1:55pm

Cellulose nanocrystal-biopolymer hybrid bioink formulation for high-resolution 3D printing of heterogeneous tissue constructs

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3D bioprinting is an additive manufacturing process which allows precise positioning of bioinks, composed of biomaterials and living cells, to create 3D tissue architectures that imitate natural tissues and organs. It is deemed the future of biomanufacturing with enormous potential impact on fundamental biomedical research, regenerative and personalized medicine. Even though 3D bioprinting technologies are advancing at a rapid pace, major challenges remain. One of which is bioink formulation. Here, we report a series of studies on a hybrid bioink system incorporating a nanomaterial, cellulose nanocrystal (CNC), and biopolymers for the high-resolution and high-speed printing of 3D tissue constructs via microextrusion. CNC is a type of rod-shaped naturally occurring nanoparticles with proven biocompatibility. Our results show that CNC-biopolymer hybrid bioinks possess promising rheological and mechanical characteristics. In particular, their excellent shear-thinning property ensures facile extrusion through a small nozzle, high print fidelity, and protection of encapsulated cells from mechanical stress-induced cell damage. By chemically modifying CNC, we investigated the effects of CNC surface charge on ink rheology and cell behavior. Two structures with well-defined biomimetic geometries were printed - bi-cellular liver lobule-mimicking constructs and layered colorectal tumor models. Cell viability, function, cell-cell interactions, and cell-extracellular matrix (ECM) interactions in the printed 3D structures were studied. Our studies offer a promising route to greatly enhance bioink formulations for printing complex architectures with multiple ECM components and cell types in sufficient resolution to recapitulate biological functions.

1:55pm - 2:05pm

Image-based Non-segmentation Finite Element Method for Mechanical Characterization of Composite Materials with Fine Inclusions

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Mechanical characterization is an important step in design of new composites and in evaluation of existing materials. Image-based finite element (FE) modeling is a powerful and efficient tool for material characterization, because it requires fewer assumptions compared with the theoretical methods and it is cheaper than the experiment methods. Composite materials with fine inclusions, for example concretes and alloys, are widely used in engineering and industry. To characterize composites with fine inclusions, voxel-based finite element modeling is too expensive especially if the design process is iterative, while a number of challenges arise when the conventional segmentation finite element method is applied [1]. First, segmentation of fine inclusions, if not impossible, is very time consuming; second, segmentation may produce topologically degenerated geometric entities that may not be mesh-able; third, if two inclusions are very close to each other, either severely distorted finite elements will be generated, or very fine elements must be used. To resolve the above challenges, we developed a non-segmentation finite element method based on Riemann sum integration. As suggested by the name, segmentation of inclusions is not required in the method. Numerical examples show that the accuracy of non-segmentation FE model is much higher than segmentation FE model, while its computational efficiency is much higher than voxel-based FE model.

Key Words: Composites, Fine Inclusions, Mechanical Characterization, Image-Based Finite Element Modeling

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2:05pm - 2:20pm

A Correlation Between Oxygen Vacancies and Elemental Analysis in Single and Binary Transition Metal Oxide Structures

Fatma Sarf¹, Emin Yakar²

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Metal oxide structures are so important to develop opto-electronic devices, catalysis systems, gas/bio sensors, solar cells and etc [1]. However, chemical growth process of metal oxides is so complicated with un-control growth rate and increasing agglomerative forms on the surface [2]. In the literature, elemental ratio (w%) is generally used to determine elements on the structure (film or nanoparticle) surface.

In this study, single (ZnO, TiO₂, SnO₂) and binary components were investigated to determine oxygen vacancies using simple elemental analysis results supported by XRD, SEM and PL measurements. With increasing oxygen elemental ratio up to 50 % and low metal elemental ratio have an impact on the agglomerative forms due to un-homogeneous solution and increasing metal(OH)₂ forms [3]. Our aim in this study, local point defects especially oxygen vacancies can correlate agglomerative forms therefore high oxygen elemental ratio.

Key Words: transition metal oxides, elemental analysis, oxygen vacancies

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2:20pm - 2:30pm

Analysis of the adhesive properties and microstructure of epoxy resin coatings modified with waste limestone powder

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Recently, civil engineering places great emphasis on the sustainable development and recycling of waste materials. The management of waste mineral powders is one of the greatest problems. These powders are derived from the extraction and processing of mineral resources and are nowadays not all re-used, but only stored in heaps. These wastes contain quartz, alumina or limestone fine powders. They are extremely hazardous in this form because they can cause pneumoconiosis, affect the nervous system in animals, pollute water and plants. On the other hand the chemical composition as well as the particle size characteristics make this byproduct an attractive additive to be used in epoxy resin coatings. The addition of waste mineral powders would reduce the total mass of epoxy resins used to make the coatings. However, the research to date on this subject contains many gaps. The epoxy resin is very harmful to the environment, especially to aquatic organisms. The use of the waste mineral powders would make the epoxy resin coatings more eco-friendly. With the above in mind, the main goal of the research was to find an amount of waste limestone powder that would improve or at least not deteriorate the pull-off strength of the epoxy resin coating. This pull-off strength is particularly important for the durability of the coating. The goal of the research was also to analyze the microstructure and chemical composition within the interphase zone between epoxy resin modified with waste limestone powder and the substrate. The tests were carried out on a 15 cm thick substrate made of C30/37 concrete. The substrate was divided into two areas with different methods of substrate surface treatment (ground surface and patched surface). On both types of the surfaces, five squares were separated for the coatings with the addition of waste limestone powder and one square for the reference sample. Before applying the coating, the morphology of the concrete surface was examined using a 3D laser scanner. An epoxy resin coating was then applied with a gradually increasing content of the selected waste limestone powder. The reference squares were covered with the epoxy resin coating without waste limestone powder. The measurements of the pull-off strength of the epoxy resin coatings were performed after the coating hardened.

using the pull-off method according to ASTM D4541. The chemical composition of the material was analyzed in the interface between epoxy resin modified with waste limestone powder and the substrate using a scanning electron microscope and X-ray micro CT. Then, the microstructure of the samples were evaluated using a micro-computed tomography. Analyzing the obtained data in ImageJ and Mathematica, graphs of fractional share of pores along the sample's height of the subsurface zone were obtained. The set goal of the research was achieved by obtaining mechanical properties at a similar level of newly formed epoxy resins.

2:30pm - 2:40pm

Design and Analysis of Epoxy Granite Reinforced with Steel Vertical Machine Center Spindle Housing

S Nallusamy, K Sujatha, M Rajaram Narayanan

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In machine tool manufacturing scenario, cast iron is widely used for different structures of machine tool manufacturing because of its good static and dynamic characteristics. To retain the structural rigidity, epoxy granite with the steel reinforcement were found to be the best replacement of cast iron for machine tool structures. Generally, machine tool structures are subjected to continuous distortions and unwanted vibrations during machining. In order to resist these effects, the structures should have better dynamic properties. Hence, cast iron has been used as structural material for structures of machine tool in case of high speed machining, higher damping properties are required. The lack of desired dynamic properties results in dimensional inaccuracies in the components. The objective of this research is to design a spindle housing made of epoxy granite reinforced with steel for a vertical machine center as a substitute for the currently used cast iron housing with the aim of improving the dynamic performance and to increase the damping potential of the structure while retaining the stiffness properties. Epoxy granite is found to provide superior damping ability which is desired in high speed machining, but possesses less material stiffness. Hence, a steel reinforced epoxy granite structure has been proposed for vertical machine center spindle housing and the proposed model has been analyzed for static structural considerations. From the analysis it was observed that, the deformation of the proposed model is less than the quantity desired. The initial reinforcement design has been arrived at from the topology optimization in the first Design Configuration (DC). The addition of reinforcements to the initial steel structure of DC-1 is reduced deformation from 230 to 6 microns in the improved steel reinforcement structure of DC-13. The reinforcement with I section in epoxy granite is found to resist deformation than other reinforcements. The improved steel reinforced epoxy granite spindle housing design possesses better stiffness compared to cast iron.

2:40pm - 2:50pm

Non-equilibrium lipid-A phosphate phases against bacterial and antiviral infections

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Lipid A-diphosphate is the abundant component of bacterial lipopolysaccharides (LPS) and found on the surface of Gram-negative bacteria outer membrane. The commensal microbiota effects the mucosal and systemic immunity, playing a potential role for microbial keystone species in autoimmunity, and rely on autonomous natural components¹ to sense their surroundings due to the variation in LPS pattern and nosocomial infections. The resistance to common administered antibiotics has resulted in a growing interest in therapies using non-toxic lipid A-phosphate or their approximants. Lipid A-phosphate and/or approximants self-assembled into body-centered and face-centered cubic liquid crystals². However, lipid A-phosphate phases driven out of equilibrium, particularly those in complex with lipid A-derivatives exhibit new structures with different properties and antimicrobial responsiveness than those at equilibrium. The crystalline phase and the liquid phase, the lipid A-diphosphate molecules exhibited two non-equilibrium phases with various degrees of translational and orientational order. A transition of lipid A-diphosphates is observed between phase-separated-fatty-acid chains and a mixed honeycomb non-equilibrium phase. The development of different 2-d faceted crystal morphologies was observed and, as growth proceeded, these faceted 2-d crystals became unstable and self-organize far from thermal equilibrium. The 2-d crystalline lipid A-diphosphate layers exhibited a pseudo-hexagonal molecular arrangement³. The development of these specific antagonistic structures creates and eliminates antimicrobial resistance, or disease-related events to booster the host defense against pathogenic invaders. For lipid A-monophosphate, rhomboid-decadehedra (Fd3m) packing was suppressed because of instability in the mean curvature between the tetrahedral and the octahedral nodes. Tetraikadodecahedra packing showed only tetrahedral nodes; the tetrahedral angle could only be retained between all edges if the hexagonal faces of the truncated octahedron were changed. The (Fd3m) multidomain structure with identical lipid A of 30°- rotated and - unrotated none-endotoxic lipid A-diphosphate layers resulted in diffraction patterns that show 12-fold rotational symmetry in the diagonal direction, for those complexes with non-identical lipid A but antagonistic lipid A-diphosphate. The spatial packing of these "spheres" was either a cuboctahedron or an icosahedron⁴, interesting samples of rhombohedral traps for oligomerization in membranes⁵.

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2:50pm - 3:00pm

3D Printing Double Network Hydrogels as Thermoresponse Nanocomposites for Dermal Drug Delivery

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Poly(N-isopropyl acrylamide) (PNIPAAm) hydrogels have shown promise for dermal drug delivery, but have been limited by the inferior strength of their swollen state. We report an exploration of using a novel P(N-isopropyl acrylamide-co-Acrylamide) system that combines Sodium Alginate and cellulose nanocrystals incorporated into the polymer, which significantly improved the hydrogel strength in the collapsed and swollen state while still allowing the temperature dependant swelling of the PNIPAAm based hydrogels. By tailoring the resin formulation for 3D printing, the lower critical solution temperature can be modified leading to printed parts with varying swelling behaviours at multiple temperatures. This study offers a promising method for the fabrication of 3D printable hydrogel structures with mechanical properties similar to cast in place hydrogels. The judicious use of solvents for 3D Printing has enabled us to print out larger parts with little change in the composition of the resin. This study offers a promising method for the fabrication of large customized hydrogel devices that can conform to complex body geometries with the possibility of dermal drug delivery by loading the hydrogel with hydrophilic drugs.

Post-2: Poster Session

Time: Thursday, 19/Aug/2021: 1:00pm - 3:00pm · Virtual location: Theatre
Session Chair: KENAN SONG

1:00pm - 1:03pm

Detecting heavy metal ions with ultra-low concentrations based on composite material incorporating reduced graphene oxide and sodium alginate

Xiaolu Zhu, Wenjie Zhao, Hao Cheng

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Heavy metal pollution is one of the most serious environmental problems. The reduced graphene oxide (rGO) with high electron transfer rate is sensitive to some external substance, and can be used to detect heavy metal ions. However, the amount of oxygen-containing functional groups contained in rGO which are used to adsorb metal ions is often not enough to meet the demand of ultra-low concentrations detection. In this study, a method for improving the metal ions detection efficacy via dispersing reduced rGO into alginate hydrogel to form a composite material as an aggregated micro-adsorber was proposed, and the composite gel material was used to detect trace heavy metal ions (Cu^{2+} , Pb^{2+} and Pd^{2+}) among microelectrodes. In this method, the alginate gel contains a large number of oxygen-containing functional groups which can enhance ions adsorption. In combination with the matched microelectrodes system with a 2 μm electrode gap, the detection of extremely small amounts of heavy metal ion solution with low-concentrations was performed. The results showed that the "gel-graphene" complex could be interpenetrated nanoporous conductive network that can be used to detect these three types of heavy metal ions with ultra-low concentrations, and the curves of volt-ampere (I-V) characteristics measured under different concentrations can be obviously distinguished. The sensitivity of this composite material to detect these 3 types of heavy metal ions is up to 40 ~ 60 dB, which is favorable to the detection of ions with ultra-low concentrations. The minimum limitation of detection concentrations is 1 pM, which is lower than the required inferior limit of ultra-low concentrations in most applications. This study offers a promising way to develop ultrasensitive electrochemical sensor for heavy metal ion detection.

1:03pm - 1:06pm

Electronic Structure and Optical Properties of Cubic and Orthorhombic CsPbX_3 (X = Cl, Br, I) Perovskite: A Theoretical Understanding from DFT Calculations

Hamid M. Ghaithan, Zeyad Alahmed, Saif Qaid, Abdullah Aldwayyan

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Caesium lead halides (CsPbX_3) perovskite has recently attracted significant attention owing to its rapidly increasing competence when used for solar cells or light-emitting diode devices. In this study, we make a comprehensive density functional theory (DFT) calculation to determine the structural, electronic, and optical properties of cubic and orthorhombic temperature-dependent phases of CsPbX_3 perovskite using the full potential linear augmented plane wave (FP-LAPW) method within the framework of the DFT, as implemented in the WIEN2k code. For this purpose, different exchange potentials: local density approximation (LDA), Perdew–Burke–Ernzerhof generalized gradient approximation (PBE-GGA), Engel–Vosko generalized gradient approximation (EV-GGA), Perdew–Burke–Ernzerhof revised for solids (PBEsol), modified Becke–Johnson generalized gradient approximation (mBJ-GGA), new modified Becke–Johnson generalized gradient approximation (nmBJ-GGA), and unmodified Becke–Johnson generalized gradient approximation (umBJ-GGA) were used. Our results on band structure indicate that the cubic and orthorhombic phases have direct energy bandgaps. Despite the large variations in their lattice constants, the two phases of CsPbX_3 possessed almost similar optical properties. This result indicates a wide temperature range of operation for CsPbX_3 .

1:06pm - 1:09pm

Bio-inspired Composite Fibers as Versatile Sensors

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One of the many challenges in materials science is to minimize the differences between naturally formed structures and manually fabricated morphologies due to the high-performance properties many bio-systems possess while synthetic materials do not have. Specifically for one-dimensional (1D) thin-diameter fibers, the control of their chemical composition and the physical phases is critical in manipulating their mechanical and functional behaviors. Our research relies on tooling engineering of the spinneret that manufactures composite fibers of different polymers and nanoparticles, leading to efficient mechanical enhancement and stimuli-responsive properties. The structure of the composite fibers mimicking the blood vessel with co-axial layers composed of polymer-nanoparticle-polymer channels. A couple of polymers have demonstrated the feasibility of using this unique structure in sensors that responded to mechanical strain (i.e., tension, compression, bending, etc.) and chemicals (i.e., liquid and gaseous volatiles). The high sensitivity to air pressure can go down to 1 psi with high consistency and the selectivity to different solvents could also be proven with low concentrations. The sensing mechanism dependent upon the electrical conductivity has also illustrated the efficiency in controlling morphologies of the nanoparticle channels, including the dispersion quality, continuity, and alignment degrees.

Key Words: bio-inspiration, functional composites, sensor

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1:09pm - 1:12pm

New Class of Crosslinker-Free Nanofiber Biomaterials from Hydra Nematocyst Proteins

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Nematocysts, the stinging organelles of cnidarians, have remarkable mechanical properties. Hydra nematocyst capsules undergo volume changes of 50% during their explosive exocytosis and withstand osmotic pressures of beyond 100 bar. Recently, two novel protein components comprising the nematocyst capsule wall in Hydra were identified. The cnidarian proline-rich protein 1 (CPP-1), characterized by a "rigid" polypyrrolone motif, and the elastic Cnidoin possessing a silk-like domain were shown to be part of the capsule structure via short cysteine-rich domains that spontaneously crosslink the proteins via disulfide bonds. In this study, recombinant Cnidoin and CPP-1 are expressed in *E. coli* and the elastic modulus of spontaneously crosslinked bulk proteins is compared to that of isolated nematocysts. For the fabrication of uniform protein nanofibers by electrospinning, the preparative conditions are systematically optimized. Both fibers remain stable even after rigorous washing and immersion into bulk water owing to the simultaneous crosslinking of cysteine-rich domains. This makes

our nanofibers clearly different from other protein nanofibers that are not stable without chemical crosslinkers. Following the quantitative assessment of mechanical properties, the potential of Cnidoin and CPP-1 nanofibers is examined in relation to the maintenance of human mesenchymal stem cells.

1:12pm - 1:15pm

Carbon composite monopole antenna: fabrication and characterization at microwaves

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Metals are commonly used as radiating elements of antennas. Nevertheless the fabrication process, the weight, and/or the sensitivity to corrosion can restrict their use. Moreover conventional antennas, attached to the surface of composite structures (mainly made of glass-fiber tissues and polyester, vinylester or epoxy resins), can impact the mechanical integrity of such panels. These problems could be circumvented by the development of new composite antennas embedded directly into the composite structures [1].

In this study, we investigate the design, the fabrication and the characterization of a planar lozenge carbon antenna embedded into a composite material panel. To this end, a single ply of a carbon-fiber tissue (woven 2/2, 385 g/m², 12 K, 370 µm-thick) with a sheet resistance $R_s = 0.15 \Omega/\text{sq}$ and a square shape (50 mm × 50 mm) acts as the radiating element (Fig. 1). This element has been embedded by infusion process into a 4 mm-thick composite laminate made of E glass-fiber tissue and polyester resin exhibiting dielectric permittivity $\epsilon_r = 4.5$ and loss tangent $\tan\delta = 0.01$ at 1 GHz. A metal antenna made of a 68 µm-thick plain copper sheet ($R_s = 2.5 \times 10^{-4} \Omega/\text{sq}$) embedded into the same glass-fiber tissue/polyester resin composite laminate has also been fabricated to serve as a reference antenna (Fig. 1). Experimental results, such as input impedance, radiation pattern, and gain of the carbon composite monopole antenna are compared with those of the metal counterpart. Both embedded antennas exhibit microwave performance strictly alike up to 2.1 GHz [2]. A wider discussion will be presented up to 6 GHz.

Accordingly, embedded carbon antennas make them suitable for a lot of wireless applications where smart skins and low profile antennas are required.

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1:15pm - 1:18pm

Development of flexible semiconductor polymer solar cell capable of environment-friendly process by improving solubility using random arrangement of donor-acceptor structure

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In this study, thiophene units are introduced into the backbone of a semiconducting polymer in either a regular (PffBT-T4) or a random (PffBT-RT4) manner to determine whether the resulting semiconducting polymers are suitable for developing efficient polymer solar cells. PffBT-RT4 has lower crystallinity than PffBT-T4 due to its random configuration. Microstructural analyses indicate that PffBT-RT4 exhibits a shorter π - π stacking distance than PffBT-T4. Since short π - π stacking distance benefits inter-chain charge transport, PffBT-RT4 shows higher space-charge-limited current mobility, and PffBT-RT4 solar cells exhibit higher power conversion efficiency

(PCE; 8.84%) than their PffBT-T4 counterparts (7.25%). In addition, PffBT-RT4 solar cells with active layers, prepared using a green solvent without any additive, show an encouraging PCE of 7.23%. Moreover, flexible solar cells based on PffBT-RT4 are much more stable during bending cycles than PffBT-T4 flexible solar cells. Therefore, this study demonstrates that the random configuration approach is a promising design strategy to realize semiconducting polymers for efficient, green-solvent processable flexible polymer solar cells

1:18pm - 1:21pm

Improved Electrical Conductivity of Carbon Fiber Composites for Lightning Strike Protection through Premixing Epoxy Resin with Carbon Nanotube Particles

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It has been decades since the first application of composite materials in industries. Carbon fiber composites, due to its light weight and high strength, are of especial interest in aerospace industries. Though the reinforcing carbon fiber materials are electrically conductive, the addition of the non-conductive resin matrix makes the overall composite laminates non-conductive which leads to the necessity for additional protection against lightning strikes. Common lightning strike protection (LSP) methods involve stacking an additional layer of copper mesh or extended metal film on top of the composite laminates which results in additional manufacturing costs and special treatment between bonding layers due to the galvanic corrosion. Our previous work was an attempt to offer a potential solution for LSP by adding carbon nanotube (CNT) additives to the resin system to improve the overall electrical conductivity of the composite laminates. In our previous work [1], Adtech 820 epoxy resin with (premixed with CNT by the manufacturer) and without the CNT additives were used to fabricate the carbon fiber composite laminates. Four-point probe tests showed a 31% decrease in electrical resistance for carbon fiber composite laminates. Due to the small test specimen sizes (6x6 inch), the simulated waveform A lightning strike with a peak current of 100 kA yielded no visible damage to our test laminates since the lightning strike was believed to be partially conducted by the grounding fixtures around the test specimens. The current work is a continuation of our previous work where varying weight ratios of CNT will be mixed with our epoxy resin to fabricate the carbon fiber composite laminates. Simulated waveform A lightning strike tests will then be conducted followed by ultrasonic scanning and SEM for damage observation, and four-point flexural test for residual strength.

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1:21pm - 1:24pm

Monolithic Inkjet Printed Multilayer Thin-film Flexible Electronics Fabrication of Conductive, Resistive, and Dielectric Polymers

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Inkjet printing (IJP), a new additive fabrication process, makes it possible to produce lower-cost large area electronics in contrast to traditional microfabrication. IJP does so by depositing thin-film layers of various inks including conductive, semi-conductive, resistive, and dielectric materials on planar substrates such as glass or polymers [1]. We have been exploring various inkjet printing approaches as the sole monolithic IJP fabrication process for preparing thin-film low-cost flexible electronics with applications to wearables, Internet-of-things, and environmental monitoring. A Dimatix Material Deposition Printer (DMP-2831, Fujifilm, Dimatix Inc., NH) was used to print these inks on glass and other flexible substrates such as polyamide (PI). The printer cartridge (10 pL droplet size) has 16-inline MEMS-based nozzles with a 20µm pitch. Silver nanoparticle inks (Metalon JS-B40G from Novacentrix, Austin, TX, with 40% loading and average particle size of 60-80 nm) were printed as the conductive layer, with a 1.8 µm thickness and a 25 mΩ/square surface resistivity on PI [2]. Polypyrrole (PPy) (Sigma Aldrich, St Louis, MO) was tested for the resistive layer. Poly(4-vinylphenol) (PVP) and CuO inks were explored as dielectric layers, with PVP outperforming with respect to superior surface smoothness and lesser micropores observed and measured by SEM and AFM. Various compositions of Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) inks were tested with limited success. The best performing composition was 4 parts of 1.1% PEDOT:PSS solution with 1 part ethylene glycol (EG) that were annealed at 180°C for 20 minutes. The contact angles on Si, PI, PVP, and Ag were 20.9°, 55.7°, 69.2°, and 20.5°, respectively, with a water contact angle on PEDOT:PSS of 19.73°. The monolithic multilayer fabrication process was successfully utilized to develop metal-insulator-metal capacitors, multilayer resistors, and flexible printed circuit boards.

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1:24pm - 1:27pm

A magnetic chiral dispersive Fresnel lens with controllable foci and dual images

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A chiral magnetic material object is a three-dimensional structure which precludes equivalence with its mirror image by rotation and translation. In this paper, we construct a magnetic chiral dispersive Fresnel lens with controllable foci and dual images, as in Fig.1, with a chiral substrate on which the grooves are etched. We intend to examine the case of a groove-in Fresnel lens with foci dependent upon the lens material parameters such as groove radii, phase refractive indices, permeabilities, permittivities, and groove depth. The use of chirality in a spherical thick lens indicates emergence of virtual and real image regimes, separated axially under dispersion based on wavelength, and also controllable anomalous image formation have been recently examined. A comparable extension is made here to a planar, chiral imaging structure based on the concept of the Fresnel lens. In particular, the case of a Fresnel lens structure with groove-in design incorporating chirality, associated dielectric loss is examined and later extended to a dispersive case with first-order material dispersion. Effects of the lens parameters on dual image formation (corresponding to right circular and left circular polarizations (RCP and LCP)), modified multiple axial images and other issues (such as dielectric losses inherent in chirality) under variable magnetic permeability and chirality coefficient κ will be discussed in this paper.

1:27pm - 1:30pm

A Multi-Channel Fast Impedance Spectroscopy Instrument for the Quality Assurance of Electric Double Layer Capacitors

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Conventional experimental methods for testing the performance of Electric Double Layer Capacitors (EDLCs) include the measurement of capacitance through charge and discharge, measurement of Equivalent Series Resistance (ESR) and measurement of self-discharge and the Equivalent Circuit Model (ECM) by Electrochemical Impedance Spectroscopy (EIS). However, the methods are not suitable for the mass production line of EDLCs since they require long time for the test and several kinds of different instruments. EIS is an attractive method to evaluate the performance of EDLCs except that it takes a long time for a single test. In this paper a fast EIS instrument suitable for quality assurance for the mass production of EDLCs is proposed. In order to reduce the time for the test, a multi-sine sweeping method is used for the EIS test and the results are analyzed by extracting the parameters of the ECM to evaluate the performance of the EDLCs. The proposed instrument is developed to have multi-channel to further decrease the time for the test with an EDLC. It is also presented as to how the extracted parameter values of the ECM can be used to evaluate the performance of the supercapacitor.

1:30pm - 1:33pm

An Efficient Green Mirror-less laser from Conjugated Polymer (PFO-co-PPV-MEHB) in Solution

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The purpose of this work is to investigate the optical and mirror-less laser properties of conjugated polymer (CO) Poly[(9,9-dioctylfluorenyl-2,7-diyl)-co-(1,4-diphenylene-vinylene-2-methoxy-5-{2-ethylhexyloxy}-benzene)] also known as [(PFO-co-PPV-MEHB), ADS125GE], dissolved in many solvents. The absorption and fluorescence spectra have been measured at various concentrations in different solvents such as benzene and toluene. The amplified Spontaneous Emission (ASE) spectra peaked approximately at 509 nm of CO PFO-co- PPV-MEHB in different solvents have obtained at suitable concentrations and pump energies. The pump source was third harmonic of Nd: YAG laser (355 nm) in transverse mode. The relationship between input pumping energy and output energy for the samples in solutions has been studied. In addition, the photochemical stability of this CO as a laser material was examined. The Time Resolved Spectroscopy (TRS) studies with sub-nanosecond resolution has been performed for CO under various pumping energy. These results have provided understanding of the excited state dynamics of CO PFO-co-PPV-MEHB and have shown that this new CO is quite efficient in the green region under Amplified Spontaneous Emission (ASE) Mode.

1:33pm - 1:36pm

Bio-sourced composites for anechoic chamber absorbers

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Today, interest in microwave-absorbing material technology has been growing where continuous and increasing efforts have also been made in the last decade aiming at developing excellent electromagnetic wave absorbers. In anechoic chambers, the microwave absorbers usually used, are made from polymer matrix, such as polyurethane or polystyrene, which are produced by the petrochemical industry [1]. These materials are pollutants and their recycling is often very complicated.

In this work, we proposed an original material made from a bio-sourced matrix, acting as a support for the absorbent load (here carbon black). In addition to the rot-proof nature of this matrix and its thermal and acoustic insulation properties, the use of this material was motivated by two other properties: its low density and its fire resistance; two properties necessary for its use in anechoic chamber.

In this work, the dielectric characterization of the materials, with different compositions in carbon black, is presented and revealed very interesting dielectric properties with regard to the intended application: namely a low permittivity associated with high dielectric

losses. The simulation of pyramidal absorbers, using measured properties, is done in order to choose the best composition for the achievement of a pyramidal prototype. The measurement of the absorber prototype showed excellent absorption performance for a normal and oblique (30°) incidences of the electromagnetic wave. Very low reflection ($\Gamma < -40$ dB) is obtained over a wide frequency range (between 3.5 GHz and 17 GHz). The prototype of Bio-sourced based absorbent also showed, for certain frequencies, better absorption performance than those of a commercial absorber with the same geometry.

1:36pm - 1:39pm

Carbon/ReS₂ composites as an attractive electrode materials in electrochemical capacitors

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Electrochemical capacitors (ECs) show to be a promising filling between fast response, high power density conventional capacitors and high energy density metal-ion batteries (MIBs). While employing carbon-based materials satisfies the demand for high power density ECs, providing high energy density without deteriorating power capabilities is challenging. Considering the energy density equation, researchers are dedicating their efforts to enhance the energy density of ECs through two different approaches: first, an integration of conductive carbonaceous components with redox-active materials such as metal oxides, hydroxides or sulphides which enhance the specific capacitance of ECs. Especially, transition metal dichalcogenides (TMDs) are placed at the centre of attention in ECs design due to the incorporation of sulphur atoms instead of oxygen, which offers higher conductivity. Second, extending the working voltage of ECs through utilizing non-aqueous electrolytes to eliminate hydrogen and oxygen evolution reactions as the result of water decomposition is proposed. TMDs are represented by the formula of MX₂, where M is a metal atom (Mo, V, Re, etc.) and X is a chalcogen atom (S, Se or Te). Recently, ReS₂ has gained significant attention due to attractive electrical, optical and vibrational properties. Additionally, its exhibit unique distorted 1T structure which gives the in-plane anisotropy in the fundamental physical properties [1]. ReS₂ is most commonly exploited in MIBs due to large interlayer spacing of 6.14 Å. The capacitor application is rarely described [2]. In this study, ReS₂ composites were prepared with different carbon materials such as three-dimensional graphene-like (3DG), carbon nanotubes or graphene nanoplatelets by hydrothermal reactions. Various structural/textural properties of these composites were characterized by scanning electron microscopy, X-ray diffraction or Raman spectroscopy. The electrochemical performance were evaluated by cyclic voltammetry, galvanostatic charge/discharge and impedance spectroscopy. Two- and three-electrode cells were employed for testing carbon/ReS₂ composites with aqueous and organic electrolytes.

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Key Words: Electrochemical capacitors, Transition metal dichalcogenides, Carbon materials, Aqueous electrolytes, Organic electrolytes

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1:39pm - 1:42pm

Combined method of thermal stabilization of electronic and energy devices based on graphene hybrid nanostructures with nontrivial capillary hydrodynamics and efficient evaporation

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Recently, interest in new methods of thermal stabilization of electronic devices based on multiphase evaporative hydrodynamics has greatly increased [1]. 2D materials, in particular graphene nanochannels and membranes, are of great interest [2,3]. The paper proposes and investigates a combined method of thermal stabilization of electronic and energy devices, which is based on graphene hybrid structures as functional materials. The method is based on nontrivial capillary hydrodynamics of the flow of working fluids, including water, through nanopores and nanochannels and effective evaporation from interfacial surfaces. High flow rates of liquids, the influence of the liquid-vapor interface, as well as the features of graphene structures (regular or random) make it possible to effectively cool the surfaces and, in part, the internal regions of devices using evaporative cooling. Models of flows in nanochannels, heat and mass transfer during evaporation, and integral models for calculating thermal management are considered. Preliminary experimental results of studying heating, vapor generation, and cooling of graphene surface nanostructures are presented. New experimental data have been obtained on the effect of the size of nanopores and nanochannels on the evaporation rate, as well as the geometric structure, as well as the addition of boron nitride and aluminum nitride nanoparticles on the evaporation rate and surface cooling characteristics. By the example of the evaporation of droplets of working fluids in a wide temperature range on various substrates, including metal mesh and graphene nanoflakes, the efficiency of the removal of high heat fluxes from heated surfaces with Joule dissipation is shown. The results of this work actually continue our earlier studies [4]. It is shown that this method of thermal stabilization is very effective, has high parameters of heat and mass transfer, and allows large heat fluxes to be removed.

1:42pm - 1:45pm

Effects of Reinforcements on 3D Printed Polymer-Derived SiOC

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Ceramic matrix composites (CMCs) are a class of structural material that are used in propulsion systems, hypersonics and nuclear power processing plants. Due to their ceramic matrix, CMCs exhibit high temperature stability at light weight (compared to metals). The reinforcements, usually in the form of fibers, particles or platelets, increase the strength and toughness of CMCs. HRL has developed a new manufacturing method that fabricates CMCs via 3D printing of reinforced polymer-derived ceramic. Using a matrix of silicon oxycarbide (SiOC) reinforced with mullite particles, we demonstrated an increase in fracture toughness from 1 MPa m^{1/2} in the neat material to >3 MPa m^{1/2} in the reinforced material. Further, we investigated the effects of an array of ceramic reinforcements, including mullite, Al₂O₃, silicon nitride (Si₃N₄), and silicon carbide whiskers, ranging from 0-40% by volume.

1:45pm - 1:48pm

Electrical Bistability studies on D.C sputtered CdZnTe (CZT) Thin films

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CdZnTe thin films were fabricated on glass substrates by D.C Sputtering Technique. X-ray diffraction pattern confirms the presence of Zinc blende CZT (CdZnTe), whereas the Scanning electron microscopic (SEM) analysis shows the 1-D morphology of the CZT (CdZnTe) films. Electrical studies shows the bistability phenomena of CZT (CdZnTe) films. The current-voltage (I-V) characteristics showed two distinct paths for forward and reverse sweep directions. Conducting Atomic Force Microscopy (C-AFM) studies also supported the bistability phenomena of the CdZnTe films. Current investigations on electrical bi-stability of the CdZnTe thin films will help to understand the defects in the photo absorber materials and the PV performance of the CdZnTe based device.

1:48pm - 1:51pm

Glass foam composites for high power microwave absorption

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Since early seventies, recycling chains of glass wastes were developed with a great success and glass containers are now widely recycled. But some types of glass, polluted with heavy metals, pose a tougher problem. Indeed, as hazardous materials, glass wastes from electronic industry (e-wastes) should be treated in specific recycling process. This is particularly the case of Cathode Ray Tubes (CRT) found in older style TV screens and monitors. Foam glass manufacture is a promising mode for re-using CRT glasses; depending on the foaming process, this cellular material combines low density, low thermal conductivity, excellent thermal stability and high rigidity. For this work, we focused our attention on EM absorptive properties of those glass foams based on cathode ray tube cullet. Inorganic additives can be used to reinforce the shielding properties in a specific spectral range. Indeed, when Carbon is used as the foaming agent, high dielectric losses are observed making of these foams a good candidate for EM absorbing applications [1,2]. In this work, we studied the impact of the glass cullet, the load rate and nature of the foaming agent on the density and the microwave behavior of glass foams. The thermal stability and the high power microwave absorbing application of these foams will be presented and discussed.

Key Words: Glass foam, electromagnetic absorption, carbon, CRT, porous structures

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1:51pm - 1:54pm

Hydrogel nanocomposite photoactuator for direct optical to mechanical energy conversion obtained by ionizing irradiation

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The incorporation of suitable nanomaterials into the stimuli responsive hydrogel matrix enables the hydrogel nanocomposites to become a key soft component of new generation of soft electronic and soft robotic devices^{1,2}. An energy transformation agent, functional gold nanoparticles and nanorods exhibit unique photo-thermal properties as a result of a surface plasmon resonance electron-phonon process and intrinsic inter-band transitions. Upon immobilization in thermo-responsive hydrogel, they induce local photo-thermal shrinking under visible light irradiation and thus enable external wireless remote control of hydrogel device and programmable photo-thermo-mechanical motion. In addition, in this way control of interface conductivity can be realized by switching hydrogel nanocomposites between electrically communicating and non-communicating states.

In this work, a soft photo/thermal reversible hydrogel nanocomposite device consisting of gold nanoparticles or nanorods embedded in poly(N-isopropylacrylamide) (PNIPAM) and poly(N-isopropylacrylamide) (PNIPAM)/poly(vinyl alcohol) (PVA) bilayer structure (in order to maximize shape changes), were developed using nanotechnology based on radiation chemistry. The key parameters deciding the actuation characteristics as well as conductivity and percolation threshold, particle diameter and shape as well as interparticle distance, can be easily tailored during synthesis using radiation processing technology. Obtained hydrogel nanocomposite device with wireless remote actuation and electrical control has great potential for light-harvesting and mechanical motion which is required for the construction of soft smart actuator systems for applications in soft robotics, for dense information storage and efficient energy conversion.

1:54pm - 1:57pm

Layer models in predicting of Composites' deformability

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Regulation and prediction of composites deformability is the important problem in providing calculated limits of structures deformations under mechanical and thermomechanical load.

Composite structure topology is discrete. But topological solution in modelling of structure deformability can include variations of elements' discreteness and infinity. Due to the structure's topological transformation by the method of flat cross-section projection the composites elements in perpendicular to load direction were represented as infinite (graphical abstract). Thus, the composite deformability layer model efficiency was supposed. Infinite elements in layer model of discrete composite structure are intermittent layers of aggregate and matrix. Aggregate is discrete element topologically represented in model as infinite in cross-load direction. The matrix layers depending on composite type can be the binder and contact to aggregate inter-transition zone (ITZ) (Type L-I), the binder only (Type L-II), the ITZ only (Type L-III).

Developing a calculation model of the composites' deformative properties, the dependence of the elastic modulus on the layer model with the number of layers $i=n$, the elastic modulus of the layer E_i and the relative thickness of the layer δ_i was proposed.

All layer model variations were researched with taking into account the type of composite structure. Analyze included heavy concrete as a type L-I, lightweight concrete as a type L-II, glassed polymer as a type L-III. Efficiency of all layer model variations were proved. It made possible to calculate elasticity modulus of cement and polymer composites depending on materials' contents in mix composition.

The layer modelling is worked out in development of entropy-topological conception of composite structure forming and analysis. The conception is aimed on definition of stress and temperature relations with composite deformability depending on mass and energy entropy. This is represented as a function of topology that includes in massive of points and coordinates massive of masses and inner chemical, physico-chemical or heat energy.

1:57pm - 2:00pm

Light-Induced Changes in the Electronic Structure of the Metal/Molecule Junctions: A Computational Modeling of Real and Designed Molecules

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Photochromic azobenzene (azo) molecular switches organized in the self-assembled monolayers (SAMs) on electrodes allow a reversible control over molecular architecture, dipole moment, and conductivity with light. New interesting and at the same time more complex systems are the SAMs consisting of azo conjugated with aromatic blocks, e.g. bithiophene (BT) [1, 2]. Such blocks affect the extent of conjugation, the dipole moment, the backbone rigidity or change the system response to the optical trigger.

Here we report a reversible light-induced configurational switching of the C-AFM tip/azo junctions (s. Figure) probed by computational modeling. In focus are the trans- and the cis-states of two molecules BT-azo (a) and azo-BT (b): the first one is studied experimentally [1, 2] and the second one represents a structural isomer of BT-azo designed by us [3].

Using DFT, we characterize the molecule/electrode coupling as a function of the chemical design, the isomerization state, and the C-AFM tip positions (b). We observe different frontier orbitals delocalization extent depending on the configuration; stronger coupling with the electrode and more pronounced charge transfer for cis-states vs. trans-states (for BT-azo: 0.20 vs. 0.04 and for azo-BT: max. 0.32 vs. 0.04 e- on gold C-AFM tip). Further, we define the energy offset between the Fermi energy and the LUMO after the light-induced switching and compare our results with literature data [1]. This research was funded by DFG (GU1510/5-1).

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2:00pm - 2:03pm

Mode Distribution and Spectral Characteristics of Chiral Thin Film Resonators under p- and s-Polarization

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Investigating the mode distribution and optical properties (such as spectral and resonance characteristics) of chiral thin films is holds out much promise in light of the rapid increase in the potential applications of thin films (including antennas, solar cells, batteries and others). The properties of these devices in the presence of chirality present greater analytical challenges. Metamaterials (which include chiral or handed materials) have been the subject of explosive interest over the past few decades because of their ability to manipulate light in both the near- and far-field zones. Also, they allow electromagnetic fields to be strongly confined within a small region, the so-called hot spot, and they are applied to varied fields ranging from molecular sensing and high-gain antennas to optical filters and smart solar cell grids [1]. Propagation across any interface containing a chiral material involves the development of left- and right-circularly polarized (LCP and RCP) modes in the chiral region. We examine chiral thin films with parallel and perpendicular polarization (p- and s-polarization) in particular to examine the differences in their characteristics as slab-type resonators. Recent work in this regard has focused mainly on the s-polarization, and has primarily demonstrated reduction and non-uniformity in mode densities and free spectral ranges. Since dielectric losses are inherent in chiral materials, their impact upon the thin film resonators

are currently under further investigation [2,3]. The work will be extended to the case of p-polarized propagation, and also include behavior under first-order material dispersion to examine the thin film resonators in different frequency bands (in particular the visible and near-infrared). Fig.1 shows the Fresnel transmission coefficients at the achiral/chiral interface (ACC) for p-polarization case. Thickness of thin films is another factor that needs to be considered to achieve the best modal fit for specific applications. It is anticipated that thin films under chirality may improve optical properties such as higher transmitted power over wider spectral bands for real-life applications.

2:03pm - 2:06pm

Biodegradation of PHBV Ternary Biocomposites in Different Environments

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The influence of different environments on biodegradation of polyhydroxybutyrate-co-hydroxyvalerate (PHBV) containing natural-based plasticizer acetyl tributyl citrate (ATBC), calcium carbonate (CaCO₃) and lignin coated cellulose nanocrystals (L-CNC) was studied. A twin-screw extruder equipped with a flat film die (0.4 mm gap size) was used for processing of ternary biocomposites and control samples. Vermicomposting, controlled laboratory thermophilic composting and freshwater biotope were used for evaluation of biodegradation. The influence of characteristics such as pH, temperature, moisture content and flow of oxygen on biodegradation rate was studied. The results of biodegradation showed an intensive degradation rate of ternary biocomposites. The addition 10 wt. % of CaCO₃ into plasticized PHBV matrix ensured 56% biodegradation after one month exposition to controlled thermophilic composting, 39% biodegradation in environment of vermicompost and 22% biodegradation in freshwater biotope. Similar characteristic but slightly slower biodegradation rates were observed for ternary PHBV biocomposites containing L-CNC (1 wt. %). In contrast, neat PHBV achieved at the same condition in thermophilic controlled composting 32% biodegradation, only 10% biodegradation in freshwater biotope and 14% weight reduction in vermicompost environment. The results showed that the highest influence on biodegradation rate of neat PHBV as well as PHBV ternary biocomposites has a temperature.

2:06pm - 2:09pm

Chiral plasmonics with freezing-directed self-assembly of nanoparticles

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Chiral plasmonic materials are desired for several photonic applications ranging from ultrasensitive biosensors to cloaking materials. However, scalable and efficient production of thin-film chiral nanoarchitectures remains challenging. We developed a new, freezing-directed method for assembling plasmonic nanoparticles using a liquid crystalline template. This approach requires: (i) synthesis of organic materials which on crystallization (freezing) form helical nanofilaments, as well as (ii) synthesis of organic ligands, which ensure chemical compatibility of metal nanoparticles with the organic matrix. To achieve chiral plasmonic materials, a mixture of nanoparticles and the organic matrix is melted to the isotropic liquid. Then, on cooling, freezing of the matrix drives the self-assembly of nanoparticles. These materials are hierarchically ordered (periodicities ranging from single to hundreds of nm), exhibit switchable structure, as well as are thermally and mechanically durable. This approach is relatively cheap since no chiral materials are required for the process, as well as universal since different types of nanoparticles (nanospheres, nanorods) can be arranged this way. We also confirmed that such materials spontaneously exhibit chiral plasmonic properties at the microscale, which can be translated to the bulk scale by the process of chiral discrimination. This research directly evidences that thin-film nanostructures with chiral properties can be efficiently prepared using freezing-directed self-assembly.

2:09pm - 2:12pm

A New Strategy for Efficient Preparation of Helical Assemblies of Gold Nanoparticles

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Achieving nanostructures with a helical geometry was found to be interesting throughout the last decades owing to their central role in natural systems, excellent structural stability, and inherent chirality. Recently, extremely dynamically developing research area has been obtaining helical assemblies of nanoparticles (NPs) that combine a helical topology with the unique plasmonic properties of NPs. Such structures open a wide perspectives due to their applications in information storage, chiral plasmonic, biosensing and metamaterial technologies[1]. So far helical assemblies of nanoparticles were prepared mainly based on the use of various type organic templates (mainly biomolecules like peptides and DNA or polymers) [2], chiral ligands and circularly polarized light. Unfortunately, these strategies are always limited to solutions and usually also to only one type of NPs. Therefore, developing new methods for achieving such architectures also in nonsolvated environments is necessary for practical application of these materials.

In our recent work [3], we develop a new solvent-free strategy in which interactions between liquid-crystalline (LC) matrix and gold NPs covered with structurally similar mesogenic ligands afford the formation of hierarchical helical nanostructures in thin films. It must be stressed that the most important advantage of the developed method, in comparison to previously described in the literature procedures, is its universality. We confirmed it by using our approach to successfully obtain helical assemblies made of nanoparticles with various size and shape. Finally it is also worth to note that unique thermotropic nature of the LC matrix gives rise to an actively tunable structure of helical nanocomposites.

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2:12pm - 2:15pm

Reconfigurable plasmonic systems based on liquid crystalline nanoparticles

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Noble metal nanoparticles show remarkable optical properties depending on the type of material from which they are made, size, shape or distance between nanoparticles, i.e. their spatial arrangement. One of the most commonly used ways to manipulate the composition of nanoparticles is self-assembly, which involves the spontaneous creation of highly ordered structures using smaller ingredients. Internal long-range organization, switchability and potential technological applications make liquid crystals ideal candidates for manipulating the self-assembly of nanoparticles into more complex crystallographic structures. They are a promising class of structures due to the fact that they enable dynamic self-assembly, thanks to the reorganization of the ligand arrangement on the surface of nanoparticles under the influence of temperature.

The main aim of this research is to obtain new types of self-assembly of plasmonic nanoparticles coated with promesogenic ligands with the use of various types of ligands and helical, liquid crystal matrices. Achieving this goal is possible thanks to the synthesis of highly monodisperse nanoparticles of distinct diameters and the introduction of organic molecules with promesogenic properties onto their surface. This type of self-assembly is particularly sensitive to the surface coverage of nanoparticles, therefore much attention is paid to its optimization. The liquid crystal nanoparticles thus obtained are mixed with suitably designed liquid crystal matrices or additional organic molecules. This step is again based on the careful selection of the amount of individual components in the mixture. In order to determine the structure of the obtained materials at individual stages of the work, a numerous analytical techniques, such as transmission electron microscopy, small angle X-ray diffraction, atomic force microscopy and UV-Vis spectroscopy were used. Obtained results indicate the possibility of preparing switchable optical / chiro-optical systems in the visible range with potential application in non-linear optics, biosensors or (chiral) metamaterials.

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2:15pm - 2:18pm

Investigation of Bioengineering Composite Bone Scaffolds

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Barium Titanate (BTO) for its superior mechanical and piezoelectric properties and hydroxyapatite (HAP) with good bioactivity due to it naturally occurring in the human bone have been widely investigated as composites for bone tissue engineering applications. However, generally, a higher volume fraction of BTO is required, to match the mechanical and piezoelectric properties of bone. Also, there is a need for biomaterial scaffolds to follow standards for testing, only 0.3% of the publications on tissue-engineered scaffolds have referenced ASTM Standards, emphasizing the need to adhere to standards for scaffold dimensions and testing methods. In this study BTO-Hap scaffolds with Poly Vinyl Alcohol (PVA) binder, fabricated and compression tested as per the ASTM D695-15 Standard, which is the prescribed method to obtain the compressive strength in ASTM F2150-19-11, the standard guide for characterization and testing of biomaterial scaffolds used in regenerative medicine and tissue-engineered medical products. Compressive strength of 110 MPa is obtained, which is in the range for the human cortical bone with only 50% volume fraction BTO thereby preserving its bioactivity with 50% HAP. The piezoelectric coefficient, d33 has been found to be 2 PpC/N after poling, where few papers have reported a similar value with higher BTO volume fractions. The improved mechanical performance with equal amounts of BTO and Hap can be attributed to the fine and homogenous grain size and smaller pores. This has been achieved by the two-step milling process prior to and after the addition of binder, before sintering the scaffolds. This study demonstrates a robust material processing technique, which can deliver scaffolds with better electromechanical properties, tested as per ASTM Standards.

2:18pm - 2:21pm Warning: The presentations finish prior to the end of the session!

Gas-phase nitrogen doping of monolithic TiO₂ nanoparticle-based aerogels for efficient visible-light-driven photocatalytic H₂ production

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Hydrogen production using abundant solar energy and semiconductor photocatalysts holds significant potential as a clean and sustainable energy system. Macroscopically sized aerogel monoliths synthesized from preformed anatase nanoparticles are promising three-dimensional photocatalysts due to their immense surface area, high porosity, translucency, and the nanoscale characteristics of the semiconducting crystalline building blocks. Recent studies showed that such titania aerogels decorated with metals are effective for gas-phase photocatalytic CO₂ reduction and H₂ production [1, 2]. However, TiO₂ nanoparticle-based aerogels remain limited to UV-driven photocatalysis due to the intrinsic wide bandgap (3.2 eV). To increase conversion efficiency from solar energy to H₂ production, visible-light sensitization is necessary. Here, we present a facile method for the doping of the aerogel monoliths postsynthetically to make them visible-light active for H₂ production. A CVD gas-phase reaction and plasma utilization at



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low temperature provided efficient nitrogen incorporation into preformed TiO_2 aerogels without affecting their initial properties. The nitridation improves the optical absorption and charge separation efficiency through an appropriate balance between doping amount and coexistent defects. In comparison to the non-doped sample, the nitrogen-doped aerogels show a significant enhancement in visible-light-driven photocatalytic H_2 production ($3.1 \text{ mmol h}^{-1} \text{ g}^{-1}$) with excellent stability over 5 days. Our approach of gas-phase nitridation of preformed aerogel monoliths offers a powerful tool to improve their properties as visible-light active photocatalysts.

FCM-4: Functional Composite Materials

Time: Thursday, 19/Aug/2021: 3:20pm - 6:00pm · Virtual location: AU 2412
Session Chair: Xiaowu (Shirley) Tang

3:20pm - 3:30pm

Thin porous PDMS membrane prepared by phase separation method and its applications for cell culture

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Cell culture inserts such as Transwell® insert with a porous membrane growth surface are useful in cell biology. Common cell culture membranes are made from polyethylene terephthalate (PET) or polycarbonate (PC), both of which are rigid polymers and not appropriate for cells that require a deformable membrane, such as lung and gut cells¹⁻². Moreover, the porosity of PET membranes are too low (< 1%) to study cell biology. While PC membranes have higher porosity (ca. 20%), cell observation is difficult due to its semi-transparency. In this study, we use a spin-casting assisted polymer blend phase separation method to prepare thin, porous, and flexible membranes for cell culture³⁻⁶. Specifically, polydimethylsiloxane (PDMS) and polystyrene (PS) were chosen for the experiment⁷. PDMS is a low elastic material which can easily perform the reversible deformation needed during observation. By selectively etching PS components into the blend membrane, a porous PDMS structure was fabricated on the membrane. Furthermore, we can adjust the thickness of the membrane, and the connectivity of PS domains by changing the concentration and blend ratio between PDMS and PS, which affects the pore size and the pore density on the final membrane. In summary, we prepared a deformable, thin, and porous PDMS membrane by a polymer blend phase separation method, which has a higher porosity compared to that of common cell culture inserts and cell culturable membranes.

3:30pm - 3:40pm

Bioinspired nacre-like composites as the next-generation of materials for safeguarding stone heritage

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The fabrication of nacre-like materials by biomimetic mineralization has gained attention as it represents an effective strategy for obtaining materials with outstanding mechanical performance. Taking the microstructure of nacre as inspiration, we are working in the development of a hybrid material composed by highly aligned calcium carbonate (CaCO₃) tablets within chitosan and cellulose multilayered films, to obtain continuous hierarchical CaCO₃ layers for stone preservation. Particular attention was paid to study the influence of varying layer thicknesses on the interface bonding in samples as well as the effect of surface functionalization of the organic layers (chitosan and cellulose) to modify wettability towards the liquid CaCO₃ precursors. Moreover, the application of the developed nacre-like composite as new surface treatments has been studied on marble lithotypes. The main results show that the role of the organic substrate, as well as the use of additives (organic compounds and polymers) are critical to obtain structural control of the mineralized layers, including their orientations, morphology, and hierarchical structure. By controlling the wettability between layers, a better control in the mineralization pathway can be induced. Because of the fracture toughness and mechanical properties of materials can be dramatically enhanced on the nanoscale, this strategy shows a huge potential to be adapted and applied to the stone conservation treatments, extending also their applicability to buildings materials of the future.

3:40pm - 3:50pm

Multifunctional Bioactive Hybrid Gelatin Microspheres Carrying Bacteriophages, bFGF and Aggregates of Mesenchymal Stem Cells

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This study attempts to prepare bioactive hybrid materials for treatment of mainly chronic wound infections like "Diabetic Foot Infection" - "DFI") and "Diabetic Foot Osteomyelitis" - "DFO") using a combinational therapy. As bioactive materials bacteriophages as antibacterial agents and basic fibroblast growth factor (bFGF) and mesenchymal stem cells (MSCs) for regeneration of both soft and hard tissue were included within the formulations. Gelatin microspheres around 50-100 micron were selected as the carrier matrices. Both basic and acidic gelatin were used to prepare microsphere hydrogels. Firstly, gelatin microgels were formed by dispersing/gelation of gelatin within an oil phase (water-in-oil dispersions). Then, these spherical gels were crosslinked using glutaraldehyde as the crosslinking agent with different relative amounts to obtain matrices with different crosslinking densities/networks. As a model target E.coli and its specific T4 bacteriophages were propagated in standard bacterial cultures. Bacteriophages and bFGF were loaded within these crosslinked gelatin microspheres. Different release rates/modes were reached/observed. MSCs were isolated from the adipose tissue from mice, cultured and 3D aggregates were formed with or without gelatin microspheres. Viabilities and metabolic activities of the MSCs in 2D and 3D forms were followed 7-14 days in proper culture conditions and compared. The benefits of 3D biohybrids (MSCs + gelatin microspheres) were approved and concluded as the methodology should be applied/continued.

Acknowledgement: E. Piskin has been supported by the Turkish Academy of Sciences as an honorary member.

3:50pm - 4:00pm

Multiscale simulation on the mechanism of debonding defect detection for concrete-filled steel tubes with piezoelectric materials

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Interface debonding between concrete and steel tube of concrete-filled steel tubes (CFSTs) leads to negative effects on their mechanical behavior and piezoelectric-lead-zirconate-titanate (PZT) has been employed as actuator and sensor to detect the interface debonding defect. In traditional structural analysis, concrete has been assumed to a homogenous materials even though concrete is a typical multiple composite comprised of coarse and fine aggregates, mortar matrix, interface transition zones (ITZs) and pores, as well as initial defects. The mesoscale structure of concrete might has an influence on the wave propagation in CFST structures. Therefore, it is necessary to further study the mechanism of the wave measurement based interface debonding detection approach considering the influence of mesoscale structure of concrete on the stress wave propagation and the response of PZT sensor embedded in concrete core or bonded on the surface of the CFST. In this paper, mesoscale numerical concrete models including circle, ellipse and irregular polygon aggregates with different distribution are employed to model concrete core of CFST and wave propagation and the response of embedded and surface mounted PZT sensor of rectangular CFST members are simulated. The effect of randomness and heterogeneity in aggregate distribution and aggregate shapes are discussed. The stress wave propagation in the cross-section of the rectangular CFST members without and with interface debonding defects under sweep frequency excitation are simulated. The sensitivity of a defined damage index based on wavelet packet energy spectrum on the sensor response is investigated in details. The results show that the mesoscale structures of concrete core has a limited influence on the PZT sensor measurement when compared with it of interface debonding defects. The results show the feasibility of the wave measurement based interface debonding defect detection approach for CFST members even the mesoscale structure of concrete core is considered.

4:00pm - 4:10pm

Sensing of Lead Using Graphene Based Chemiresistive Sensor

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Heavy metal contamination in water by mercury, lead, cadmium and arsenic has always been a serious threat to our environment as these elements are toxic and have a tendency to accumulate in our body and cause long term disorders. Accurate detection of these poisonous heavy metals is necessary and the most widely used techniques in this domain are inductively coupled plasma-mass spectroscopy (ICP-MS), and atomic absorption spectroscopy (AAS). However, these techniques are costly, require bulky instrumentation and real time detection is not possible. We have developed a simple and cost-effective chemiresistive sensor using reduced graphene oxide (rGO) as the sensing material for detection of lead (II) in aqueous medium. The sensor was prepared by first making a thin film of graphene oxide and the film was converted into reduced graphene oxide by thermal and chemical treatment. Selectivity towards lead was improved by using beta cyclodextrin. The sensor response, i.e. the change in resistivity in the presence of PbNO₃ solution was recorded in the range of 1 to 600 ppm. This study shows considerable change in the resistivity of the sensing medium in the presence of salt solution. We were able to obtain around 60% change in resistivity for 50 ppm and around 15% change for 10 ppm for PbNO₃ within 15 minutes. This sensor device offers practical solution for field detection of lead in case of industrial waste water and along with that further studies are to be undertaken for improving the detection limit of the sensor.

4:10pm - 4:20pm

A vibration assisted nano-syringe structure using Carbon Nano Tube

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Carbon nanotubes (CNT) having a needle-like geometry with a small radius and good mechanical properties have been attracting much attention as a material for nano syringe in biomedicine and biotechnology area. However, for its practical medical applications, there are a few obstacles that need to be improved: (i) In the process of penetrating the skin (phospholipid bilayer), the needle may cause damage in the skin tissue, (ii) the needle-like geometry of CNT may be clogged by the phospholipid bilayer structure and (iii) the fluidic drug in nano-syringe may get high flow resistance. To overcome these issues, the authors utilized the oscillation characteristics of the multi-wall CNTs. The previous studies reported the multi-wall CNT oscillation characteristics are very sensitive to their initial geometrical or thermodynamical conditions. Therefore, the authors varied initial parameters, such as chirality and external energy source, to get an optimized CNT nano-needle model using molecular dynamics simulations. It is confirmed that the proposed CNT model effectively reduces the puncture force during the lipid bilayer insertion process. In the drug delivery procedure, the effect of vibration on flow resistance is also confirmed. These results presented in this study demonstrate that CNT has great potential in the nano-biomedical industry as a novel syringe material.

4:20pm - 4:30pm

Application of new TF-SPME coating materials based on deep eutectic solvents for preconcentration of trace amounts of organic contaminants in environmental sample analysis

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Nowadays, targets in analytical chemistry include the monitoring and assessment of the state of the environment and the determination of trace amounts of contaminants, often in variable and complex matrices. It is also important to introduce solutions in both analytical instruments and procedures following the principles of Green Analytical Chemistry. These principles assume shorter time and less laborious analytical procedures, automation and miniaturization of measuring devices, as well as the elimination or reduction of used volatile organic compounds, and the reduction of waste.

Therefore, the technique of solid-phase microextraction (SPME) proposed by Pawliszyn and co-workers in 1990 is so popular among analysts. In the SPME technique, analytes are adsorbed on a fiber coated with appropriate materials. From the point of view of Green Analytical Chemistry, the solvent-free nature of adsorption, as well as the use of little or no solvent in the desorption stage and the possibility of multiple uses of the fiber are important.

Currently, the SPME technique is developing mainly towards the composition of new coating materials as well as various geometries of devices [1]. The coating materials can also be applied to a flat surface, e.g. as a thin film on a stainless steel mesh that acts as a support/fiber in the SPME. This related technique is known as thin-film solid-phase microextraction (TF-SPME).

The main aim of the present study is the preparation of new coating materials based on deep eutectic solvents and their application for the TF-SPME technique. The scope of the study includes the design and then synthesis of new deep eutectic solvents (DESs) in various molar ratios of hydrogen bond donor (HBD) to hydrogen bond acceptor (HBA), which is carried out taking into account their selective use for the extraction of analytes with defined polarity. Next, stable coating materials based on DESs are applied to form a thin film on a stainless steel mesh, directly or by sol-gel technology.

The TF-SPME technique with new coating materials was used to isolate and preconcentrate trace amounts of organic contaminants such as parabens, aldehydes, pesticides followed by their chromatographic analysis.

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Key Words: Deep Eutectic Solvents, Thin Film Solid Phase Microextraction,

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4:30pm - 4:40pm

Effect of Composite Filler on Mechanical Properties and Material Homogeneity in Solid Tire Vulcanization for Trolly

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Filler is one of the most important materials used to make various types of rubber vulcanizate. The filler in the rubber compound-making process acts as an active filler to improve the mechanical properties of the vulcanisate, and acts as a volume-increasing filler to reduce production costs. The filler composites used in this study are specifically for solid trolly tires which are commonly used to move goods within the airport area. Solid tire rubber vulcanisate in this study used a filler composite consisting of silica as an active filler, kaolin and CaCO₃ as a volume enhancer. The loading of filler composites on the rubber matrix in this study varied from 50 to 65 phr. The manufacture of rubber composites for solid tires is carried out through a process of chewing, mixing natural rubber with synthetic rubber Butadiene Nitrile Rubber, compounding, and vulcanization. The vulcanization process is carried out at a temperature of 150 °C for 20 minutes. The data from the test results before and after aging show that the composite filler ratio has an effect on specific gravity, hardness, and abrasion resistance. The homogeneity of the material was scanned using a scanning electron microscope (SEM). The scan results show that the distribution of the material on the rubber vulcanized matrix is influenced by the ratio of the filler material. To see the functional groups of solid tire rubber vulcanisate used Fourier transform infrared spectroscopy (FTIR).

4:40pm - 4:50pm

Evaluation of Polymeric Ionic Liquids-Chitosan Beads as An Innovative Adsorbent to Trace Multitarget Analytes from Waste water

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Pyridine based polymerized ionic liquids were successfully utilized for the first time with the combination of chitosan (Cs) and graphene oxide (GO) as an innovative adsorbent to trace multitarget analytes from waste water. A very simple and easy system (peristaltic pump) was exploited to produce sphere-shaped minor and fine beads. Consequently, the following three samples were prepared and characterized: Cs-beads, poly (4-vinylpyridine) octyl bromide/Cs-beads, poly (4-vinylpyridine) octyl bromide/Cs/GO-beads. Infrared Spectroscopy (IR) confirmed the chemical connections present among all constituents. Scanning Electron Microscopy (SEM) revealed the porous nature of adsorbent. Beads was tried for the elimination of heavy metals and organic pollutants from waste water. Arsenic and copper ions were designated as model pollutants to address heavy metals, methylene blue and naphthalene were also carefully chosen pollutants to report organic family. Batch adsorption technique was used. Inductive Coupled Plasma-Optical Emission Spectroscopy (ICP-OES) was used for the analysis of the remaining quantity of arsenic metal, copper ions were detected through atomic absorption spectroscopy. UV-visible spectroscopy and high-performance liquid chromatography were used to

analyzed dye and naphthalene uptake, respectively. Polymeric ionic liquids-based composites beads showed good adsorption behavior towards metal ions. The adsorption capacity of beads towards copper ions uptake was around 98 %. The chosen adsorbent was poly (4-vinyl pyridine) octyl bromide/Cs/GO-beads. The results encourage the integration of poly (4-vinyl pyridine) octyl bromide with other polymers and fillers for further improvement in related applications.

4:50pm - 5:00pm

High frequency response of biomass-derived carbon in aqueous electrochemical capacitor

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Electrochemical capacitors are the devices for reversible energy storage. They are characterized by high power output owing to non-faradaic type of charge storage, while having only limited energy density. This parameter is governed by both capacitance (C) and cell voltage (U). The cell voltage is essentially dependent on the specific electrolyte type (aqueous, organic, ionic liquid), while the capacitance is mainly influenced by the active surface area of carbon. However, it has been already shown that additional contribution to the capacitance is achieved thanks to the pseudocapacitance originated from heteroatoms present in the electrode material, mainly nitrogen, but other, like sulfur, oxygen and phosphorus are also reported.

In this work, we demonstrate the high capacitance of biomass-derived carbon based on nitrogen-rich adenine precursor obtained via soft-templating method. The performance of two-electrode system (with 1 mol L⁻¹ Li₂SO₄ electrolyte) equipped with a reference electrode is compared to the commercially available carbon Kuraray YP-50F. The interesting parameters of the carbon is not only the superior gravimetric capacitance comparing to commercial carbon (100 F g⁻¹ vs. 130 F g⁻¹), but also the outstanding frequency response shown in Fig. 1. The extensive studies aiming at the correlation of physicochemical properties of these carbons with electrochemical performance will be provided.

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5:00pm - 5:10pm

Synthesis and characterization of a new highly absorbent material based on carboxymethyl guar gum as an alternative to conventional absorbents in disposable hygiene products

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Superabsorbent polymers (SAPs) are cross-linked networks of hydrophilic polymers with a high absorption capacity of water and aqueous solutions. They have attracted a lot of attention due to their exceptional properties. This has made them ideal for a wide range of valuable applications in medicine, agriculture, and industry in general. However, their greatest application is as a liquid-absorbent material in disposable hygiene products. Disposable baby diapers, feminine sanitary napkins, and incontinence protection for the personal care market are rapidly improving. This market is growing rapidly in regions with very high birth rates and aging demographics, such as developing countries, where superabsorbent materials are among the materials most in daily demand in the market. These days, most commercially available superabsorbent products are made from petroleum-based vinyl monomers, therefore, they are not biodegradable and environmentally friendly. In response to this challenge, environmental protection laws are beginning to encourage the use of renewable and biodegradable materials because of their low production cost and biodegradability. In this context, superabsorbent polymers of natural origin derived from polypeptides and polysaccharides have undergone chemical and biochemical modifications to improve their ability to absorb and retain large quantities of liquids.

The objective of this research is to develop a new highly absorbent material capable of absorbing a large amount of water, based on a guar gum chemically modified and reinforced with a mineral charge. The chemical structure of the material has been characterized by Fourier Transform Infrared Spectroscopy (FTIR), Thermogravimetric Analysis (TGA/DTA), Scanning Electron Microscopy (SEM), and X-ray Diffraction (XRD). The swelling performance of the new material was also investigated. The centrifuge retention capacity (CRC) is about 30 g/g and the absorbency under load (AUL 0.3 psi) is not inferior to 14 g/g in saline solution (0.9 % w/w). Furthermore, a comparison of the swelling capacities of the synthesized material with commercial SAPs extracted from hygiene products showed that the performance was somewhat similar, which favors the use of this natural-based material.

5:10pm - 5:20pm

Synthesis and characterization of hydroxyapatite-reinforced chitosan composite hydrogel for bone tissue regeneration

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reinforced chitosan composite hydrogel have emerged as promising biomaterials for tissue engineering applications[1]. This is a relatively new and emerging interdisciplinary field that applies the knowledge of bioengineering (the life sciences) and the clinical sciences towards solving the critical medical problems of tissue loss and organ failure. The aim of this work was to fabricate an injectable porous scaffold material hydroxyapatite (HAp)/ chitosan composite hydrogel and investigate its potent application in bone tissue engineering[2]. However, the hydroxyapatite was successfully synthesized from eggshells waste and confirmed by various chemical's techniques[3].



Hydroxyapatite was successfully synthesized using eggshell waste as a raw material. Eggshell waste and orthophosphoric acid were co-precipitated for 2 h at an ambient temperature. The pH of the solution was adjusted to 10 using ammonium hydroxide. Then, 10–30 wt% of hydroxyapatite was loaded into the chitosan film. Furthermore, the hydroxyapatite (HAp)/chitosan (CS) composite has been confirmed by scanning electron microscopy (SEM), thermogravimetric analysis (ATG), X-ray diffraction (DRX), Fourier transform infrared spectroscopy (FTIR) and the swelling behavior of the composite was observed in phosphate buffer saline solution.

Finally, the hydroxyapatite (HAp)/chitosan (CS) composite presented good excellent properties as a tissue engineering material.

5:20pm - 5:30pm

STUDY OF MECHANICAL AND CHEMICAL PROPERTIES STABILITY OF INNER TUBES EXPOSED TO GAMMA RADIATION

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Nowadays, car tires are not provided with inner air or tubeless, pointing toward a technical evolution. Nevertheless, trucks tires even use at present inner tires, composed almost fully by a synthetic material, which ensures either a good potential for air constraint or longer periods for inspection of tires pressure. Inner tire is located inside the tire which does not have any extra sealing in the wheel to withstand compressed air. It is designed to resist to expansion of these elements, inside common tires. This rubbery and vulcanized coating has chemical and physical characteristics which enable it to bear a very high air pressurization, avoiding leakages while protects tire outer frame. Inner tires models are exposed to higher temperatures and pressures that contribute to accelerate abrasion. This work aims to the study of mechanical properties changes of an inner tire used in trucks, after gamma rays exposure, in order to promote further material recycling. Ionizing radiation choice was due to its capacity to modify materials structure and properties besides its applicability for rubbers recycling/recovery. For samples characterization, non-irradiated and irradiated at 5, 10, 15, 20, 25 and 30 kGy, there were accomplished following tests: tensile and elongation at break, hardness, thermal ageing and CHN elementary analysis. It was observed a decrease in mechanical properties for irradiated samples at doses higher than 20 kGy

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5:30pm - 5:40pm

Design of a lightweight fiberglass stalk for a 'fan palm' camouflaged cellular tower

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In the current era, mobiles phones have become a necessity for many people worldwide. The increasing mobile phone usage has fuelled demand for a large number of cellular towers. However, people do not want a telecommunication tower erected in their locality as it ruins the landscape. So, the telecommunication companies have come up with the idea of camouflaged cellular towers. Despite being a brilliant idea, the existing 'fan palm' camouflaged cellular towers in Mauritius are not widely appreciated because they are far from resembling natural trees and are not durable enough. The artificial 'fan palm' stalk is made of high molecular weight polyethylene and the lack of flexibility of the structure makes it prone to crack formation and even breakage under bending or twisting caused by strong winds. Failure of the stalk can cause casualties and also damage the antennas, thus affecting signal transmission. In this study, the redesign of the stalk of such a camouflaged tower has been inspired by a natural 'fan palm' stalk. Given its high modulus of rupture and good tensile strength, the RF transparent fiberglass material has been chosen for the stalk. The geometrical features of a natural 'fan palm' stalk, such as cross-sectional area and shape, have been replicated in the artificial one such that the latter behave naturally. The stalk should be flexible so that it can swing like a natural one. This has been achieved through shape optimization and weight reduction of the stalk. A 3D model of the stalk has been created in Solidworks and the stress induced under cyclonic wind conditions has been analyzed by performing a structural static analysis in Ansys Workbench. It has been observed that the nature-inspired shape of the stalk has a huge impact on increased durability and flexibility of the structure.

5:40pm - 5:50pm Warning: The presentations finish prior to the end of the session!

Functional materials for smart plastics, and beyond: Morpholino-poly(piperazinyl-morpholinyl-triazins)

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Plastics, the polymer composites, perhaps the smartest materials ever created in recent times have enabled quantum leaps possible in our evolution and life-style, in shortest possible period of history; their worst curse being that they are too good to be true. However, there are some major issues with plastics such as a) visible and invisible degradation, of both polymer and the ingredients, in inevitable melt-processing, (largely underestimated), b) potential fire hazard while-in-use, being basically solid fuels and c) ultimate disposal of, after-the-use, as waste (not being properly addressed)1-3.

MCA technologies GmbH in Switzerland has developed an environmentally friendly technology that on one hand provides safety in processing and imparts a sustainable fire-safety-in-use to plastics, and on the other hand, it enables their ultimate environmentally friendly disposal as waste, coupled with simultaneous generation of usable energy4.5. The knowledge & experience thus gained from energy extraction of waste plastics could provide guidelines to increase the efficiency of energy production and reduction of emissions from combustion fuels in general. The technology is also intended to safeguard against open burning of plastic waste that can lead to flashover and forest fires.

The chemistry and the working mechanism principles of the technology, applicable as well to alleviate the fire-hazard of lithium ion batteries, will be presented at the symposium.



AAAFM

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Functional Materials

Materials For Life

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Key Words: Polytriazines, Plastic Processing, Safety-in-use, Waste Disposal. Combustion Fuels, Energy Storage

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EPMM-4: Electronic, Photonic and Magnetic Materials

Time: Thursday, 19/Aug/2021: 3:20pm - 6:40pm · Virtual location: AU 2410

Session Chair: Yang-Ki Hong

3:20pm - 3:30pm

Spectroscopic and Magneto-optic Properties of Tb³⁺ and Mn²⁺-doped CdS Q-dots in Silicate Glass for Faraday Rotation

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We demonstrate the control of Q-dot-scale structures of CdS, Mn²⁺-doped CdS and Tb³⁺-CdS in a silicate glass for magneto-optical applications. The microstructural properties of Q-dot glasses were characterized by X-Ray diffraction (XRD), Field Emission Transmission Electron Microscopy (FETEM), UV-Visible-NIR spectroscopy and room temperature Photoluminescence (PL) spectroscopic techniques. The FETEM of the CdS QD-glass structure analysis demonstrates that the size distributions of CdS, Mn²⁺-doped CdS, and Tb³⁺-doped CdS Q-dots were in the sub 10 nm nm. The size distribution analysis of Q-dots was found to be consistent with the determination of Q-dot size using the line-broadening measurements in XRD and average Bohr radii estimation using the UV-visible spectroscopy. The XRD and FETEM analyses also confirm that the Mn²⁺-ions dissolve in the hexagonal CdS structure, consequently the estimated values of lattice parameters of hexagonal CdS are smaller than that for undoped CdS Q-dots. Detailed PL spectroscopic analysis, when excited with 380 nm source, demonstrate the characteristic emission in the 560-750 nm for undoped and 500-725 nm for Mn²⁺-doped Q-dot CdS glasses, respectively. The changes in line-shapes of PL spectra were also investigated as a function of the heat treatment temperature, from which the process of nucleation and growth of Q-dots were also analyzed and the influence on PL spectra were characterized. The magneto-optical Faraday rotation measurements were studied at room temperature with magnetic fields up to 360 mT for all Q-dot containing glass samples. Significantly, we observed a large increase in the value of Verdet constant from 6.2 to 12.0 degree/T-cm in glass samples with Mn²⁺-doped CdS[1]. The demonstration of large Verdet constant in Q-dot silicate glasses with sub Tesla field paves the path for engineering range magneto-optical devices for photonics, spintronics and sensors applications, in which the polarization of photons may be controlled with low-intensity magnetic field in glass waveguides and optical fibres.

3:30pm - 3:40pm

Physical Properties of Nano-crystalline TiO₂ thin films prepared by Thermal Evaporation

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We have successfully grown the nano-crystalline TiO₂ thin films on BSG substrates by thermal evaporation technique. XRD patterns revealed a mixture of anatase and rutile phases. The origin of the mix phase confirms the source material itself. The FESEM image of the TiO₂ films exhibits high-quality nano-crystalline structure with uniformly distributed identical grains of ~22 nm size. The samples show significant transmission in the entire spectrum, which slowly increases from the visible side (45%) to the NIR side (85%). The thickness of the films is approximately 92 nm. The refractive index of the sample displayed a rapid decrease in the UV region, while in the visible and IR regions, it recorded a slow decline. Transmission data also confirmed the nano-crystalline growth of the films. PL spectra exhibited many luminescence peaks, which suggest potential applications and also confirmed the bandgap observations obtained from the transmission spectrum.

3:40pm - 3:50pm

Organic Functional Materials Derived from Rigid Ladder-Type Molecules and Macromolecules

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Conjugated ladder-type molecules and macromolecules represent an intriguing class of organic compounds featuring rigid pi-backbone and promising potential applications as functional materials. In such a structure, the coplanar molecular conformation facilitates the delocalization of not only molecular orbitals, but also possible charges, excitons, and spins, leading to synergistically ensembled properties of the entire conjugated system. A rigid backbone, meanwhile, imposes a low entropy of the system and a high energy cost to disrupt such a favorable conformation, ensuring the robustness and persistence of coplanarity. From a supramolecular and material point of view, coplanarity and rigidity often promote strong intermolecular electronic coupling and reduce the energy barrier for the transport of charges, excitons, and phonons, affording advanced material properties in bulk. This talk describes our effort in the design, synthesis and processing of novel conjugated ladder-type organic materials. By taking advantage of their unique constitutional and conformational structures, we demonstrate the promising applications of this class of materials in terms of thermoresponse, electronics, Pauli paramagnetism, gas adsorption thermodynamics, etc.

Key Words: ladder polymer, pi-conjugation, organic electronics, gas adsorption, thermoresponsive materials, Pauli paramagnetism

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3:50pm - 4:00pm

Magnetic impregnation on K0.5Na0.5NbO3 through multiferroic doping

Umi Nuraini¹, Fitriana Fitriana¹, Malik Anjleh Baqiya¹, Pinit Kidkunthod², Masatsune Kato³, Suasromo Suasromo¹

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The (K0.5Na0.5)NbO3 composition was prepared through solid state reaction, while doping material BiFeO3 through sol-gel self-combustion method. The magnetic impregnation occurred in conjunction with dopant dissolve into the matrix, the method adopts standard procedure of ceramic processing, calcination at 5750C for 6 hours then sintering at 1100°C for 2 hours. The characterization includes X-ray diffraction (XRD), X-ray spectroscopy (XAS), and superconducting quantum interference device (SQUID) magnetometer. Crystal structure of the studied material was tetragonal at room temperature. XANES Fe K-edge analysis revealed that the absorption energies consist of quadrupole transition $1s \rightarrow 3d$ (t_{2g} and e_g) and dipole transition $1s \rightarrow 4p$ (p_{π} and p_{σ}). These energies were higher than that of Fe2O3 suggesting the oxidation state of Fe was a mixture of 3+ and 4+, thereby creating defects in the structure $[\text{Fe}]_{\text{Nb}^{4+}}$, $[\text{Fe}]_{\text{Nb}^{3+}}$ and influencing magnetization. The paramagnetic (K0.5Na0.5)NbO3 become para-ferromagnetic after dopant BiFeO3 dissolved in the matrix. It is believed that the origin of magnetic moment is 3d unpair electrons of Fe occupied in octahedron BO6 and influenced by the existence of ferromagnetic ordering interaction $\text{Fe}^{3+}\text{-O}^{2-}\text{-Fe}^{4+}$ of side by side octahedron.

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4:00pm - 4:10pm

Functional property of adjacent narrow thin film strips with inclined uniaxial magnetic anisotropy

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A magnetic momentum in a magnetic thin film behaves as if it is restricted in a 2-D sheet, due to the strong demagnetizing force along the thickness direction of the film. The momentum in the film clustered by the exchange force and forms a certain pattern of magnetic domain. A formation and variation of the pattern of magnetic domain is dominated by magnetic energy which is affected by the external field, the anisotropy energy, and the 2-D shape of the film. In this study, we utilize the quasi-2D property of magnetic thin film to a functional device such as a sensor having a memory function or a switched device using its specific magnetic phenomenon.

Our previous research shows that a narrow rectangular shaped thin film element with inclined in-plane easy axis in 70 degrees has a typical characteristic of magnetic domain transition. The transition phenomenon also can be controlled by a normal magnetic field. In this report, we apply this controlling method to parallel line adjacent many-body configuration of elements having the typical transition property in each element. There is mutual magnetic interaction existing within the many-body elements. A high frequency permeability as a function of the domain transition of the many-body element is also investigated. It is important for realizing a high-density device using this phenomenon.

4:10pm - 4:20pm

Elastic properties assessment in the multiferroic BiFeO3 by pump and probe method

Pierre Hemme¹, Philippe Djemia², Pauline Rovillain³, Yann Gallais¹, Alain Sacuto¹, Anne Forget⁴, Dorothée Colson⁴, Eric Charon³, Bernard Perrin³, Laurent Belliard³, Maximilien Cazayous¹

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Multiferroics that show cross-correlation between electric and magnetic properties are promising materials for future hybrid computational architectures that transform information from one state into another, such as spin excitations into charge, phonons or photons. Among multiferroics, bismuth ferrite (BiFeO3) is the prototypical multiferroic with outstanding properties and has shown

application potential in fields as diverse BFO-based nanoelectronic devices and spintronic. It leads also to spectacular THz electromagnetic wave generation and photostriction properties. The prospects for applications in this area such as optically triggered piezotransducers require a perfect knowledge of the elastic properties of materials. The knowledge of the elastic properties of BFO is desired for the integration of BFO in nano-electronic devices.

Combining pump-probe experiment at the picosecond time-scale with density functional theory and calculations of theoretical velocities, all the C_{ij} elastic constants have been determined in an unprecedented effort.¹ Our methodology necessitates only one single crystal whereas more are needed in case of Brillouin scattering.

We implement pump-probe experiment at the picosecond time-scale on BFO single crystal to measure the sound velocities of the (quasi)-longitudinal and two (quasi)-transverse acoustic waves along three independent directions of the (110) surface. Moreover, one surface wave and one longitudinal wave propagating perpendicular to the surface have been detected.

From a set of initial elastic constants calculated by the density functional theory, the resolution of the Christoffel equation gives access to first theoretical velocities. The minimization of the difference between the experimental and theoretical velocities allows determining all six independent C_{ij} elastic constants. The comparison of the directional dependency of experimental and theoretical sound velocities enables identification of the longitudinal, fast and slow transversal acoustic modes and the generalized Rayleigh surface wave.

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4:20pm - 4:30pm

Observation of enhanced conductivity in n type nano crystalline diamond implanted with nitrogen and phosphorus

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Diamond is known as an 'ultimate engineering material' because it possesses extreme properties suitable for various applications including highest thermal conductivity, high hardness, transparent over a wide range of frequencies, highly incompressible, and highly resistant to chemical reactions. Doping of diamond further multiplies its area of research, for example, through nitrogen doping and boron doping, the bandgap of diamond can be engineered. Resistivity and grain size of diamond films can be tuned to suit various applications in the field of electronic devices. Quantum qubits can be generated in diamond where quantum information processing can be efficiently realized. However, Diamond (bandgap, $E_g = 5.47$ eV) suffers from an asymmetric doping problem and thus, n type doping is relatively difficult compared to p type. Introduction of boron atoms into the sp^3 bonded carbon network of diamond creates impurity levels at 0.36 eV above the valence band maximum (VBM). When heavily doped with boron, the impurity levels aggregate into a band. Beyond a critical concentration for the insulator to metal transition (IMT), impurity band merges with the valence band. Therefore, at high boron concentration ($\sim 4.5 \times 10^{20} \text{ cm}^{-3}$) diamond becomes a superconductor^{1,2,3,4}. This has been well studied by many groups. Our group is currently working on realizing n type diamond by ion implantation with nitrogen and phosphorus which are the potential n type donors. Doping nitrogen to a level to induce insulator to metal transition has been a big challenge which we have succeeded and we have observed that doping with nitrogen and phosphorus in ultra nanocrystalline, nanocrystalline and even single crystal diamond has brought enhanced conductivity along with insulator to metal transition which was clearly evident in transport properties. The development of high quality n type diamond thin films with such high conductivities has potential applications in diamond based electronic devices and quantum computing.

4:30pm - 4:40pm

Revisiting Mossbauer-Spectroscopy Characterization of Magnetic Materials

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There are three kinds of hyperfine interactions observed in a Mossbauer spectrum. Mossbauer spectroscopy gives quantitative information on the isomer shift (δ), electric quadrupole splitting (Δ or QS), the magnetic hyperfine field (MHF), and Curie or Neel temperature (TC or TN) of iron-based magnetic materials. The δ (Coulomb interaction between protons of the nucleus and s electrons) is related to iron oxidation state, spin state and bonding properties, the Δ (interaction between the nuclear quadrupole moment of the ground or excited state and an inhomogeneous electric field at the nucleus) related to the degree of crystal distortion, thereby magneto-crystalline anisotropy energy (coercivity), and MHF (interaction between the nuclear magnetic dipole moment and a magnetic field) associated with the magnetic moment (saturation magnetization) and inequivalent crystallographic sites, i.e., sublattices.

Mossbauer applications include studying the structure and magnetic properties of nanocrystalline and amorphous materials, core-shell magnetic materials, the interfacial region between ferromagnetic nanocrystallite and amorphous matrix, substituted sites, and magnetic phase transformation. In this paper, we will introduce basic Mossbauer spectroscopy and a detailed interpretation of the Mossbauer spectrum to obtain quantitative magnetic properties.

4:40pm - 4:50pm



A New Boundary Element Formulation and Analysis of Fractional-Order Three-Temperature Nonlinear Generalized Thermoelastic Problems of Functionally Graded Magnetic Thermoelectric materials

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The main aim of this article is to introduce a new fractional-order theory to contribute for increasing development of technological and industrial applications of functionally graded magnetic thermoelectric materials. This theory, called three-temperature nonlinear generalized thermoelasticity of functionally graded magnetic thermoelectric materials (FGMTM). In order to guide the current research field to the development of new functionally graded materials (FGM), we should successfully implement the computerized numerical methods that are used to solve and simulate difficult nonlinear FGM problems. The governing equations of the proposed theory are very complex to solve experimentally or analytically because of very strong nonlinearity. To overcome this, we need to develop new numerical techniques for solving such equations. Therefore, we propose a new boundary element method (BEM) formulation for solving the theory's governing equations. Due to the advantages of the BEM solution such as treating problems with complex shapes that are difficult to treat with traditional methods and does not require the discretization of the internal domain. Also, it requires low CPU usage and low memory storage. Therefore, the BEM is suitable for treating a wide range of advanced FGMTM applications. The numerical results are presented highlighting the effects of the effects of magnetic field and graded parameter on the thermal stresses in FGMTM. The numerical results also confirm the validity and accuracy of the proposed formulation and solution technique.

4:50pm - 5:00pm

Progresses in Developing Micro-Multilayer Multifunctional Electrical Insulation (MMEI) System for High Voltage Applications

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Development of the novel patented high voltage insulation system, namely micro-multilayer multifunctional electrical insulation (MMEI) was continued particularly for the future hybrid or all electric aircraft applications. Initially, the concept and feasibility of the MMEI system was successfully demonstrated with its exceptionally high dielectric breakdown voltage, reaching 91% highest increase over the Kapton® PI film alone at the same overall thickness when the multilayer structure of the Kapton® PI films and binder layers such as PFA was optimized in terms of individual film thickness and layer configuration, Figure 1. Overall, MMEI structures outperformed any other SOA polymer insulation materials or commercial system such as Teflon-Kapton-Teflon (TKT). Since then, further optimizations and improvement of the system were pursued with specific emphasis on multifunctionalities such as moisture blocking, partial discharge (PD) resistance, durability, etc. Efforts have been also continued to identify the controlling mechanisms for the major improvement in dielectric strength of the MMEI structures via 3-dimensional dielectric failure mode analysis, Figure 2. At the same time, significant progresses have been made in scaling up the MMEI structures and assessing their commercial applicability and manufacturability in full-scale 3-dimensional prototypes of electrical components, such as power cables and bus bars. Overall progresses on the MMEI development to date will be presented in this paper.

5:00pm - 5:15pm

Strainoptronics: 2D materials with a twist

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Strainoptronics is an emerging concept that allows to manipulate and hence engineer a plurality of materials properties such as the bandgap, mobility, and Schottky barrier height for example. 2D materials are especially utilizable for strainoptronics given their low dimensionality leaning to a strong (2-4%) 'strainability'. In this presentation, I will share our latest explorations and device demonstrations including (a) an efficient TMDC photodetector at 1550nm wavelength on Silicon PICs [1, see right figure], (b) engineering the Schottky barrier height and reducing the bandgap by 200meV [2], and (c) showing scaling-length-theory based slot detectors with a potential for high gain-bandwidth-product photodetectors [3]. In detail, in integrated photonics, specific wavelengths are preferred such as 1550 nm due to low-loss transmission and the availability of optical gain in this spectral region. For chip-based photodetectors, layered two-dimensional (2D) materials bear scientific and technologically-relevant properties such as electrostatic tunability and strong light-matter interactions. However, no efficient photodetector in the telecommunication C-band has been realized with 2D transition metal dichalcogenide materials due to their large optical bandgap. Here, we demonstrate a MoTe₂-based photodetector featuring strong photoresponse (responsivity = 0.5 A/W) operating at 1550 nm in silicon photonics enabled by strain engineering the 2D material. Unlike Graphene-based photodetectors relying on a gapless band structure, this photodetector shows a ~100X improved dark current, enabling an efficient noise-equivalent power of 90 pW/Hz^{0.5}. Key Words: tensile strain, work function, 2D materials, MoTe₂, photodetector, SOI.

5:15pm - 5:25pm

WGM lasing from Sm 3+ ZnO micro spheres fabricated by laser ablation technique

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Whispering gallery modes (WGMs) from dielectric micro cavities possess very small mode volume and high quality (Q) factor, are find applications in nonlinear optics, micro lasers, ultra sensitive molecular sensors, etc. Being a wide bandgap material ($E_g = 3.37$ eV), ZnO is one of the suitable hosts for rare earth (RE) ions. To realize RE specific 4f emissions in the visible spectral range, interband levels are created in the bandgap of ZnO by doping with suitable RE ions [2]. In the present study highly smooth and crystalline Sm³⁺:ZnO microspheres were synthesized by laser ablation process using sintered targets in air. Sharp WGM

resonances in the visible range $\sim 550\text{--}750\text{ nm}$ are observed due to the coupling of $\text{Sm } 3+ f f$ transitions namely, $4 G_{5/2} \rightarrow 6 H_{J}$ ($J=5/2, 7/2, 9/2$ and $11/2$) to the WGMs of the $\text{Sm } 3+:\text{ZnO}$ microcavity. The resonances are found to be lasing above low threshold and have Q factor of the order of 10^3 . These results could be useful for light emission and sensing applications which operate in the visible spectral range.

5:25pm - 5:35pm

Elastic, Magnetothermal and Magnetocaloric Effect of YFe_3 and HoFe_3 Compounds

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We report on the temperature and field-dependence of the magnetothermal properties and magnetocaloric effect in YFe_3 and HoFe_3 compounds. The mean-field theory and the ab initio calculation, using the Density Functional Theory (DFT) as implemented in the Wien2k code, were used. The calculations of the magnetization, magnetic heat capacity, magnetic entropy and the isothermal change in entropy ΔS_m were performed using the two-sublattice model of the mean-field theory. For calculating the lattice, electronic specific heat and the corresponding entropies, and subsequently the adiabatic change in temperature ΔT_{ad} , we performed the ab initio calculation to determine the Debye temperature Θ_D and the density-of-states at E_f . The bulk and shear moduli of YFe_3 are in the 95-236 GPa range, the average speed of sound is $\approx 4167\text{ m/s}$, and the Debye temperature is $\approx 500\text{ K}$. The trapezoidal method was used to calculate ΔS_m , in fields up to 60 kOe, and at temperatures up to and beyond the Curie temperature for both compounds. The maximum values, in a 60 kOe, of ΔS_m for YFe_3 and HoFe_3 are about 1.3 and 0.25 J/mol. K respectively. The temperature and field dependences of the magnetothermal properties and of ΔS_m and ΔT_{ad} show that the ferro/ferrimagnetic to paramagnetic phase transition, in these two compounds, is a second-order-phase-transition (SOPT). The Arrott plots and the universal curve were calculated to provide further checking the type of magnetic phase transition involved in these compounds.

5:35pm - 5:45pm

General Trends in Core-shell Preferences for Bimetallic Nanoparticles

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Core-shell nanoparticles have gathered much attention of the scientific community owing to their potential applications in various fields including biomedical imaging and catalysis. Predicting core-shell preference¹⁻³ is, however, still largely based on a few experimental observations and limited theoretical studies, and hence development of new core-shell nanoparticles is normally built on a trial-and-error approach. Here we present general trends of core-shell preferences for 45 bimetallic nanoparticle systems studied by molecular dynamics (MD) and Monte Carlo (MC) simulations. Simulations were performed using LAMMPS code and the embedded-atom method (EAM) potentials were employed for simulating the interactions between atoms in the bimetallic nanoparticle systems composed of 10 metals; Ag, Cu, Au, Pd, Fe, Co, Ni, Pt, Al, and Mo. In order to quantify the core-shell preference, the MD/MC results were analysed to identify surface atoms using the alpha-shapes method. The core and shell compositions of the preferred equilibrium structures of bimetallic combinations were then used to categorize each combination into one of four different types depending on the level of core-shell tendency: mixed, core-shell, highly segregated core-shell, Janus-like. The categorized MD/MC results were also analysed using principal component analysis (PCA) and linear discriminant analysis (LDA) to determine the primary factors that dictate core-shell tendency. Eight possible factors were considered, and cohesive energy and atomic radius are found to be the two primary factors that have an 'additive' effect on the segregation level and core-shell preference in the bimetallic nanoparticles studied. In the majority of the investigated combinations, the element with higher cohesive energy has smaller atomic radius and tend to occupy the core. Highly segregated structures (highly segregated core-shell or Janus-like) are expected to form when both the relative cohesive energy difference is greater than $\sim 20\%$ and the relative atomic radius difference is greater than $\sim 4\%$. However, when the element with higher cohesive energy has larger atomic radius, the core-shell tendency decreases. The general trend observed in the current study^[1] can be used as a guide in nanoparticle synthesis methods in which heat-induced surface segregation phenomena play an essential role, and in predicting the equilibrium structures of bimetallic nanoparticles.

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5:45pm - 5:55pm

Imperceptible energy harvesting device and biomedical sensor based on ultraflexible ferroelectric transducers and organic diodes

Barbara Stadlober¹, Andreas Petritz^{1,2}, Esther Karner-Petritz^{1,2}, Takafumi Uemura^{2,3}, Philipp Schöffner¹, Teppei Araki^{2,3}, Tsuyoshi Sekitani^{2,3}

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Energy autonomy and conformability are essential elements in the next generation of wearable and flexible electronics for healthcare, robotics and cyber-physical systems. This study presents ferroelectric polymer transducers and organic diodes for imperceptible sensing and energy harvesting systems, which are integrated on ultrathin ($1\text{-}\mu\text{m}$) substrates, thus imparting them with excellent flexibility. It was found that these ultraflexible ferroelectric polymer transducers (UFPTs) develop improved ferroelectric properties through thermal annealing resulting in an increased crystallinity. After poling the remnant polarization reaches values up to 70 mC/m^2 in close correlation with the crystallinity and the decrease of the dielectric constant. Simulations show that the sensitivity of ultraflexible ferroelectric polymer transducers can be strongly enhanced by the use of the ultrathin substrate. The ultrathin substrate furthermore

allows the mounting of the transducers on 3D-shaped objects and the stacking in multiple layers. Indeed, UFPTs have improved sensitivity to strain and pressure as compared to devices on rigid thick substrates with values up to 15 nC/N; they have a fast response (< 20 ms/N) and an excellent mechanical stability with a bending radius down to 40 μ m. Accordingly, they can be used as imperceptible wireless e-health patches for precise pulse and blood pressure monitoring. For harvesting biomechanical energy, the transducers are combined with full wave organic rectifier circuits made of ultraflexible organic diodes. These diodes are based on organic thin film transistors with short-circuited drain and gate and are fabricated on the ultrathin substrate as well. The diodes have an excellent on/off ratio up 107 and a transition voltage around 0V. Transducers, diodes and ultrathin capacitors (needed as storage elements) were further combined to form an imperceptible, 2.5 μ m thin, energy harvesting device with an excellent peak power density of 3 mW/cm²–3.

5:55pm - 6:05pm

Terbium doping and luminescent activation effects on the optical and luminescent properties of aluminum zinc oxide thin films

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Rare-earth doped wide bandgap (WBG) semiconductors have attracted great attention as efficient luminescent materials for optoelectronic applications, such as photon downshift, down- and up- conversion systems, a new generation of low voltage light-emitting devices, non-contact luminescent temperature sensors and photonic structures. However, the luminescence activation of rare-earth ions is yet to be successfully achieved in transparent conductive oxide (TCO) films, such as indium tin oxide (ITO) or aluminum zinc oxide (AZO) which also have a WBG and often form part of those structures and devices. Such optically active TCOs would therefore be advantageous for these applications. Our work focuses on the production and characterization of terbium (Tb) doped AZO thin films, keeping a high optical transmittance in the visible region and exhibiting Tb³⁺ characteristic luminescence. The effect of Tb doping on the optical and luminescent properties was investigated for different post-deposition annealing conditions. Films were produced on silicon and fused silica substrates by radiofrequency magnetron co-sputtering employing high purity AZO and Tb targets. Samples were annealed post-deposition between 200°C - 1000°C in air or argon ambient. Optical transmittance, spectroscopic ellipsometry, photoluminescence (PL), cathodoluminescence (CL) and energy dispersive X-ray spectroscopy experiments were made after each annealing step. As grown and annealed samples revealed characteristic Tb³⁺ emission. Absorption coefficient, band gap and Urbach energies were estimated using computational methods and models developed in our group. PL and CL results suggest an indirect excitation mechanism of activated Tb ions. To further assess this possible mechanism, temperature dependent PL experiments, ranging from -190 °C to 300 °C, were carried out on representative samples. It is proposed that excitation energy is transferred from bound excitons to activated Tb³⁺ clusters. This is tentatively modeled using a spherical potential well, as well as a tight-binding one-band approximation approach for a short-range charge trapping process and subsequent formation of bound excitons to rare earth ions clusters.

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6:05pm - 6:20pm

The Quest for new Thin Films and Heterostructures Multiferroic at Room Temperature

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Multiferroic are a special class of smart materials that exhibit both ferroelectric and magnetic properties and have generated great interest for a variety of applications, ranging from spintronic devices to novel photovoltaic devices, and from cryogenic-free highly-sensitive magnetic sensors to innovative non-volatile memories. However, obtaining materials with ferroelectric and magnetic properties that are sufficiently strong and robust at or above room temperature for potential integration into novel devices remain elusive. The search for thin films and heterostructures of new materials with good multiferroic properties at room temperature remains a major challenge, especially since the existence of good ferroelectric and magnetic properties does not guarantee the existence of a strong coupling between them.

Consequently, several strategies have been pursued in the quest for thin films and heterostructures of novel multiferroic materials with good multiferroic properties at room temperature. Some of these strategies will be presented, exemplified by different thin layers and heterostructures that have been synthesized and that are multiferroic at room temperature. The characterization of the structural and functional properties of these room temperatures multiferroic thin film systems, including at the ultralocal scale, will then be presented and discussed in detail. Finally, some perspectives on this fascinating class of materials and their potential applications will be presented.

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6:20pm - 6:30pm Warning: The presentations finish prior to the end of the session!

Three-dimensional plasmon-generating nanostructure for surface- enhanced Raman scattering and plasmon-enhanced fluorescence detection

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In this study, silver nanowire 3D random crossed-wire woodpile (3D-RCW) nanostructures were designed and prepared. The 3D-RCW provides rich “antenna” and “hot spot” effects that are responsive for surface-enhanced Raman scattering (SERS) effects and plasmon-enhanced fluorescence (PEF). The optimal construction mode for the 3D-RCW, based on the ratio of silver nanowire and control compound R6G, was explored and established for use in PEF and SERS analyses. We found that the RCW nanochip capable of emission and Raman-enhanced detections uses micro levels of analysis volumes. Consequently, and SERS and PEF of pesticides (thiram, carbaryl, paraquat, fipronil) were successfully measured and characterized, and their detection limits were within 5 μM –0.05 μM in 20 μL . We found that the designed 3D plasmon-enhanced platform cannot only collect the SERS of pesticides, but also enhance the fluorescence of a weak emitter (pesticides) by more than 1000-fold via excitation of the surface plasmon resonance, which can be used to extend the range of a fluorescence biosensor. More importantly, solid-state measurement using a 3D-RCW nanoplatform shows promising potential based on its dual applications in creating large SERS and PEF enhancements.

Key-3: Keynote Session-3

Time: Friday, 20/Aug/2021: 8:00am - 10:00am - Virtual location: Theatre

Session Chair: Richard B. Kaner

8:00am - 8:40am

Water-based and biocompatible 2D Inks: from Fully Inkjet Printed Heterostructures to Biomedical Applications

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Solution processing of graphene [1] allows simple and low-cost techniques such as inkjet printing [2, 3] to be used for fabrication of heterostructures of arbitrary complexity. However, the success of this technology is determined by the nature and quality of the inks used.

In this work we show a general formulation engineering approach to achieve highly concentrated, and inkjet printable water-based 2D crystal formulations, which also provide optimal film formation for heterostructure fabrication [4]. Examples of all-inkjet printed devices, such as large area arrays of photosensors on plastic [4], programmable logic memory devices [4], strain sensors on paper [5], capacitors [6] and transistors [7] will be discussed.

In addition, our approach allows easy production of defects-free and biocompatible graphene flakes with positive or negative charge [4,8-10], which can be used to elucidate the effect of surface charge on cellular internalisation and other biological interactions.

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8:40am - 9:20am Warning: The presentations finish prior to the end of the session!

Stimuli-Responsive Nanoparticles Controlled by Supramolecular Machines and Caps for Biomedical Imaging and Drug Delivery

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The subjects of this talk are multifunctional mesoporous silica nanoparticles controlled by stimuli-responsive coverings over the pore openings for imaging and drug delivery in cells and in vivo. The nanoparticles are designed to 1) trap therapeutic molecules inside of the nanocarriers, 2) carry therapeutics to the site of the disease with no leakage, 3) release a high local concentration of drugs, 4) release only on command – either autonomous or external, and 5) kill the cancer or infectious organism. The most important functionality is the ability to trap molecules in the pores and release them in response to desired specific stimuli. Two types of noninvasive external stimuli will be discussed: high intensity focused ultrasound (HIFU) and oscillating magnetic fields. They will be compared with internal biological stimuli such as pH changes and redox potential changes. Stimuli-responsive caps including supramolecular systems, “snap-top” disassembly, and thermo-sensitive systems will be described. Nanoparticles containing anticancer drugs in the mesopores are taken up by cancer cells, and stimulation of the caps releases toxic molecules and kills the cells. Both reusable and completely reversible nanovalves will be described. Activation of these nanodevices in solution, in living cells, and in animal models will be discussed. Image-guided drug release stimulated by HIFU and imaged by MRI will be presented, and applications of stimuli-responsive drug release for treatments of cancers (including pancreatic and breast) and of intracellular infectious diseases (including tuberculosis and tularemia) will be discussed.



EPMM-INV-1: Electronic, Photonic and Magnetic Materials

Time: Friday, 20/Aug/2021: 8:00am - 10:00am · Virtual location: AU 2410

Session Chair: Qibing Pei

8:00am - 8:15am

Van der Waals heterostructure by stacking engineering

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Van der Waals heterostructure by stacking engineering

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Van der Waals (vdW) materials have attracted extensive attention because of their impressive stable properties at atomic thickness. The interlayer vdW interaction in the 2D material uniquely allows building a vdW homo/hetero-structure by a layer-stacking means without the need for lattice matching,^{1, 2} superior to the conventional solid interface grown in vacuum generally suffering from various perturbations, such as defects,³ lattice mismatch,⁴ and atomic interdiffusion.⁵ Here, we demonstrate the novel spintronics properties, such as ferromagnetic-antiferromagnetic exchange bias effect in vdW heterostructures by stacking engineering, compared to that in conventional materials. Our work provides a path for the exploration of other novel physics such as quantum anomalous Hall effect, topological superconductivity in two-dimensional heterostructure materials.

Key Words: Spintronic materials; Van der Waals; stacking heterostructure

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8:15am - 8:30am

Van der Waals structures make near-IR quantum cascade lasers

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Quantum cascade lasers (QCLs) constitute a leading source of coherent radiation in the mid-infrared region. However, their performance outside this region remains unsatisfactory. Indeed, there are currently no QCLs in the near-Infrared (near-IR) region. I propose that a superlattice of atomically thin layers held together by van der Waals forces can operate as a compact and powerful room-temperature near-IR QCL emitting at wavelength 1.66 μm . It can compress over 100 stages within 0.5 μm . The electric field required for operation is about $3 \times 10^6 \text{ V/cm}$, while the lasing threshold current density is about 22.4 kA/cm^2 depending on parameters. Rate equation analysis shows that the peak power per unit volume can reach over $0.1 \text{ mW}/\mu\text{m}^3$ in continuous wave (c.w.) operation. Unlike most existing QCLs, our device is p-type working with holes designed with an unusual injector.

8:30am - 8:45am

Atomic Imaging Functional Heterostructures and Interfaces by Phasing Coherent Bragg Rods for Quantum Materials

Hua Zhou

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Ubiquitous in a wide range of nature processes and technologies, a subtle modification (e.g. structurally, chemically, or electronically) near an interface can have a decisive effect on properties of the collective as well as each individual. A compelling case manifesting such subtlety is oxide heterostructures and heterointerfaces exhibiting fascinating emergent behaviours due to numerous combinative contributions of atomic structures and chemistries, which can be effectively harnessed for the design of advanced materials for information and energy applications and accelerating materials integration into advanced devices. Surface/interface X-ray scattering from modern synchrotron sources integrated with phase retrieval direct methods provides a very powerful toolkit to decipher the interfacial subtlety. This is essential to our ability to provide a quantitative and realistic description of the interfacial boundaries by which to engineer properties of functional interfaces using atomic structure-driven design principles in a reliable and controlled manner.

In this seminar, I will firstly give a brief introduction of how to obtain atomic mapping of multifunctional heterostructure and heterointerfaces with sub-Ångström resolution by phase retrieving coherent Bragg rods, wherein complete atomically structural

information hidden, in particular on the COBRA method in combination with the difference map algorithm achieving unprecedented speed of convergence and precision. In the following, I will demonstrate some science cases in the exploration of oxide heterostructures and heterointerfaces for quantum information applications by applying the direct method, such as revealing structural motifs responsible for various quantum states (e.g. 2DEG/2DHG, interfacial superconductivity, polar metal and 2D skyrmions) adjacent with heterointerfaces, catching structural perturbations in response to internal and external electric fields, and depth-resolved mapping oxygen-octahedral connectivity network essential with incipient ferroelectricity of heterostructures. In the end, I will give a short commentary on emerging opportunities in X-ray studies of multifunctional interfaces and heterostructures of quantum materials enabled by the exciting advancements towards ultimate storage rings, in particular with enhanced high-energy, coherence and ultrafast capabilities.

8:45am - 9:00am

A fistful of chemico-physical parameters crucial for ¹H-NMR relaxation: the effect of size, shape and coating in iron oxides core-shell nanoparticles

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An increasing awareness about novel medical applications of smaller, inorganic-based nanoparticles, possessing unique properties at the nanoscale, has led to a burst of research activities in the development of "nanoprobes" for diagnostic medicine and agents for novel, externally activated, therapies. In this research field, magnetic nanoparticles (MNPs) are prominent due to fundamental peculiar properties which make them particularly appealing to materials and biomedical applications.

In particular, much attention was devoted to MNPs useful as agents for Magnetic Resonance Imaging (MRI), Optical Imaging (OI) and Magnetic Fluid Hyperthermia (MFH), carriers for drugs and vectors for molecular targeting. The possibility to collect images of the regions where the MNPs are delivered through MRI and eventually OI (if functionalized with a luminescent molecule), is joint to their use under radio-frequency fields, with frequency of the order of 100 KHz, which causes a local release of heat directed to tumour cells (the MFH effect), possibly inducing their death. By such materials, theranostic agents can be obtained. On the other hand, in the field of drug delivery and molecular targeting, few examples of reproducible experiments using superparamagnetic nanoparticles are actually present in literature. Thus, the applications of MNPs to nanomedicine is currently of growing interest in the world.

The main objectives of my research group in the last decade was to contribute to the knowledge of physical mechanisms at the basis of MNPs used in biomedicine (especially MRI) and to propose some novel systems in strict collaboration with different research groups of chemists and biologists. I will present a mini-review of different case studies [1-4] where I show how the chemico-physical characteristics of MNPs are strictly correlated to their properties and can be partially interpreted with the most famous heuristic model [5] used in literature for NMR relaxivity profiles.

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9:00am - 9:15am

Controlled concentration and transportation of nanoparticles at the interface between a smooth substrate and droplet

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Controlled concentration of nanoscale materials on the surface of a smooth substrate without vibration excitation mechanism and micro channels, and transportation of the concentrated nano material on the surface, have large potential applications in the fabrication of nano sensors and electrodes, decoration and assembly of nano materials, etc. However, implementation of these two nano manipulation functions by one single device has been a big challenge. Here we report a method to concentrate nanoparticles at an arbitrary location at the interface between a smooth substrate and water droplet, and to transportation the concentrated nano material freely at the interface. It employs the acoustic streaming, which is generated by a micro manipulating probe (MMP) vibrating linearly above the substrate. SiNPs can be concentrated under the MMP at a desired location, forming a round spot of nano materials with a diameter up to 230 μm . The concentrated nano material can be transported through an arbitrary path at the interface by shifting the device, and has little change in the size and shape during the transportation. The dependency of acoustic streaming field around the MMP on device parameters is clarified by numerical computation and verified by experiments.

9:15am - 9:30am



Carbon fibers based epoxy foam composites: from dielectric characterization to electromagnetic absorption application

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Due to the rapid development of electronics and telecommunications, protection against electromagnetic waves has become an active area of research, and the intensification of protective materials usage is reflecting the market needs and the great demand of such products. The form and composition of electromagnetic absorbers are various and depend on the application under consideration. The typical absorbing materials used in the market have either flat or pyramidal forms. Pyramidal absorbers made of flexible polyurethane foam impregnated with a solution containing carbon particles are currently the most used materials for anechoic chambers. However, the carbon particles deposited inside the pores of the foam remain dangerous for human health due to their high volatility and nanometer sizes. This paper presents an alternative electromagnetic absorbing material developed from rigid epoxy foam and carbon fibers. The rigid foam was chosen because it can be machined with a complex geometry in order to enhance the absorption performances. Furthermore, our process enables the complete embedding of the fibers which prevents any leak. For this study, several composites of epoxy foam loaded with carbon fibers with length between 0.1 mm and 3 mm were achieved. Dielectric properties (permittivity and dielectric losses) of these materials were measured in 2 – 18 GHz frequency range. Therefore, numerical simulations of the reflection coefficient were performed to estimate the absorption performances of a pyramidal absorber and also a new designed geometry made of epoxy foam loaded with 0.5 %wt. of 3 mm carbon fibers. The simulation results showed remarkable performances: the reflection coefficient reached the mean value of – 45 dB. The measurement of prototypes in anechoic chamber confirmed the excellent performances with an equivalent even better reflection coefficient than the most used commercial absorber.

Key Words: Carbon fibers, composites, electromagnetic absorption, anechoic chamber, dielectric properties

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9:30am - 9:45am

Transformative piezoelectric enhancement of electrospun P(VDF-TrFE) by nanoscale dimensional reduction and their potential bio-applications

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Despite the significant potential of organic piezoelectric materials in the electro-mechanical or mechano-electrical applications that require light, flexible, and biocompatible materials, the intrinsically low piezoelectric performance as compared to traditional inorganic materials has limited their full utilization. We demonstrate that dimensional reduction of poly(vinylidene fluoride trifluoroethylene) (P(VDF-TrFE)) at the nanoscale by electrospinning, and furthermore with an appropriate thermal treatment, induces a transformative enhancement in piezoelectric performance. Specifically, the piezoelectric coefficient (d_{33}) reached up to -108 pm/V, approaching that of inorganic counterparts. Electrospun mats composed of these thermo-treated 30 nm nanofibers with a thickness of 15 μ m produced consistent peak-to-peak voltage of 38.5 V at a strain of 0.26%. This exceptional piezoelectric performance was realized by the enhancement of piezoelectric dipole alignment and the materialization of flexoelectricity, both from the synergistic effects of dimensional reduction and thermal treatment. Our findings suggest that dimensionally controlled and thermally treated electrospun P(VDF-TrFE) nanofibers provide an opportunity to exploit their flexibility and durability for mechanically challenging applications while matching the piezoelectric performance of brittle, inorganic piezoelectric materials. By fine tuning their properties, we demonstrate their potential applications pertaining to nano-biotechnology/medicine in drug release, nerve regeneration, and a wearable device.

9:45am - 10:00am Warning: This presentation lies outside the session time!

Development of High-Frequency β -Ga2O3 Field-Effect Transistors Aiming for Applications to Harsh-Environment Electronics

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Beta-gallium oxide (β -Ga2O3) has recently gained significant attention as a next-generation power electronics semiconductor owing to its extremely large bandgap energy of 4.5 eV [1] and high breakdown electric field of over 8 MV/cm [2]. The saturation electron velocity (V_{sat}) in β -Ga2O3 is theoretically predicted to be greater than 1e7 cm/s [3], indicating that β -Ga2O3 field-effect transistors (FETs) are attractive for not only power switching but also high-frequency wireless communications and high-speed logics. In this talk, we will present our development of submicron-gate β -Ga2O3 FETs for applications at high temperatures and/or under strong radiation [4].

We fabricated highly scaled β -Ga2O3 FETs with various gate lengths (L_g) from 50 to 1,000 nm on unintentionally doped Ga2O3 epitaxial layers grown on Fe-doped semi-insulating Ga2O3 (010) substrates by molecular beam epitaxy. The n-type Ga2O3 channel with $Si = 4.8 \times 10^{18} \text{ cm}^{-3}$ was formed by Si-ion implantation doping. T-shaped gates were fabricated on an Al2O3 gate dielectric by 100-keV electron-beam lithography and liftoff processes. The source-to-drain distance and the gate width were 2 and 100 μ m, respectively.

Superior RF small-signal characteristics of a current-gain cutoff frequency (f_T) of 9 GHz and a maximum oscillation frequency (f_{max}) of 27 GHz were achieved at $L_g = 200 \text{ nm}$. Note that the f_{max} is a record value for Ga2O3 FETs. These high-frequency characteristics are sufficient for applications at frequencies up to 10 GHz, which have been widely used for wireless communications in present-day society.

Delay-time analysis based on the L_g dependence of fT was also performed to investigate an effective electron velocity (V_e) in the Ga₂O₃ channel region under the gate. The V_e of about 2×10^6 cm/s was experimentally extracted from a slope of a fitting line on the total delay time versus L_g plot; the value was consistent with the V_{sat} theoretically predicted.

This work was supported in part by the Strategic Information and Communications R&D Promotion Program (SCOPE) of the Ministry of Internal Affairs and Communications, Japan.

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10:00am - 10:15am Warning: This presentation lies outside the session time!

Single nanowire chemoresistor as a gas sensor to assess food quality

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The ability to assess the quality of food throughout the production and distribution chain, from producer to consumer, is very important. This allows to reduce food waste, increase the efficiency of the system and avoid problems of food poisoning and consequent health costs. To make this possible you need sensors that are tiny and cheap, but that can assess the quality of food quickly and accurately. Chemoresistive sensors are ideal for this task: they are micron sized, easy and inexpensive to manufacture and read, and are sensitive to a wide range of volatile compounds.

In this specific case, a single tin oxide nanowire was used to evaluate the state of freshness of mackerel fish (*Scomber scombrus*) over time. The single nanowire sensor measures the concentration of total volatile basic nitrogen (TVB-N), which collects dimethylamine, trimethylamine and ammonia (produced by fish-degrading bacteria). The response of the sensor to the TVB-N was compared with the bacterial population measurements, resulting well correlated with the total vital counts (TVC). The resistive nanosensor therefore proves to be ideal for having a first estimate of the quality of the mackerel (stored at room temperature or in the fridge), which can be obtained non-invasively and in a few seconds

EPMM-INV-2: Electronic, Photonic and Magnetic Materials

Time: Friday, 20/Aug/2021: 8:00am - 10:00am · Virtual location: AU 2412

Session Chair: Rizwan Raza

Session Chair: Mohsin Ali Badshah

8:00am - 8:15am

Glial interfaces: biomaterials, devices and approaches to trigger and monitor the “other brain”.

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Evidence produced over the past 30 years showed crucial roles of glial cells, called astrocytes, in brain function and dysfunction and moved the neurocentric vision of brain science towards a more holistic perspective. Since astroglial reactivity is a major cause of failure of brain implant performance, the study of astrocytes/material interaction can also drive knowledge on engineering safe and long-term stable biosensors and bioelectronic neural interfaces.

A major pitfall in the study of astrocytes is that technologies used to understand their mechanism, structure and function are limited or adapted from those engineered for neuronal cells. In this context, the goal of our study is to validate bioelectronic materials, devices and biophotonic approaches to selectively probing and sensing astrocytes physiology (namely ion channels, water channels and calcium signalling) and to understand their role in brain physiology and pathology. In this respect, the presentation will overview the results obtained on: 1) using of bioelectronic devices, based on silicon nanowire, graphene and organic semiconductor, that allows stimulation and recording of astrocytes calcium signalling and voltage membrane oscillations, 2) the potential of photonic and optical approaches to trigger selective calcium signalling in astroglial cells 3) the use of nanostructured interfaces that allow for generating a model of astrocytes in vitro mimicking morphological structure and function they show in-vivo.

The presented results evidenced that glial interfaces might help in unveiling unexpected role of astrocytes in brain cognitive function and can provide novel path for therapeutical neuromodulation approaches.

Supported by AFOSR projects ASTROMAT; ASTRONIR, 3D NEUROGLIA, ASTROLIGHT

Key Words: Astrocytes, graphene, organic semiconductor, biopolymers, glial interfaces

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8:15am - 8:30am

Inducing room temperature Superparamagnetism in iron, manganese and cobalt oxide Spinel nanostructures by Nickel incorporation

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Inducing room temperature Superparamagnetism in iron, manganese and cobalt oxide Spinel nanostructures by Nickel incorporation

First row transition metal oxides with spinel structure are interesting materials due to their excellent magnetic and catalytic properties, which have also been utilized as electrode materials in energy storage devices.¹ Although most of these metal oxides have antiferromagnetic behavior, substitution with other transition metal ions transforms them to ferromagnetic. Due to inherent ferrimagnetic nature and multivalent metal ion constitution, these metal oxide nanostructures are highly attractive for heterogeneous catalysis. However, inducing superparamagnetism at room temperature would make them even attractive for biomedical applications such as in magneto-hyperthermia.² Magnetic behavior of a metal oxide is defined by its lattice spin arrangement, which in turn, depends on its composition.³ In this talk, we will present the results of structural and magnetic characterization of some metal oxide nanostructures of spinel structure (NixFe3-xO4, NixCo3-xO4 and NixMn3-xO4) to demonstrate the possibility of inducing superparamagnetism in them through Ni incorporation. Based on structural analysis, we propose reasonable cation distributions in the binary metal oxides nanostructures that can explain their observed magnetic behaviors. We also demonstrate that a phase transition from antiferromagnetism to superparamagnetism can be induced in these nanostructures by incorporating a certain amount (mol fraction) of nickel ions in their lattice. Induction of room temperature superparamagnetism in these metal oxide nanostructures is the result of the combination of two factors: (i) the strong preference of Ni²⁺ ions to occupy the octahedral sites of the spinel lattice, and (ii) smaller effective magnetic moment of the Ni²⁺ ions compared with Co^{2+/3+}, Mn^{2+/3+} and Fe^{2+/3+} ions. Octahedral site preference energy (OSPE) of the ions in the lattice is a key parameter to explain these results.

Key Words: Spinel, Superparamagnetism, Nanostructures.

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8:30am - 8:45am

Atomic-scale surface characterization of (opto)electronic III-V semiconductor nanowire devices

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Semiconductor nanowires are promising candidates for next generation (opto)electronic and photovoltaic devices, such as solar cells made of InP pin-junction nanowires [1] or tunnel FETs based on InAs-GaSb axial nanowire heterostructures [2]. III-V semiconductor nanowires with superior charge carrier mobility and direct bandgap can be epitaxially grown on silicon substrates without interfacial defects, enabling quantum-size effects with a large flexibility in combining different materials. Due to the small size and high aspect ratio of nanowires, their properties are to a significant extent determined by surface effects. Therefore, atomic-scale surface and interface characterization is crucial for understanding and improving the performance of nanowire-based devices.

Here, I will present our toolbox for complementary and atomic-scale surface characterization of III-V semiconductor nanowires, based on scanning tunneling microscopy and spectroscopy (STM/S), atomic force microscopy, and synchrotron X-ray imaging and spectroscopy methods. We map heterostructures between different doping levels [3], materials [4,5], or different crystal phase [6-8], where we correlate the surface structure and local electronic properties across the interfaces of axial nanowire heterostructures. Recent efforts include in-operando and in-situ studies, where we investigate nanowires during device performance [3,4] or while their surface becomes modified [8].

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8:45am - 9:00am

Color Tuning of Single-Fluorophore Emission via Polymerization-Mediated Charge Transfer

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Organic light-emitting materials have attracted much attention due to their great potential for various applications, such as organic light-emitting diodes, fluorescent sensors, bioimaging, and disease diagnostic. For practical use, it is essential to design the light-emitting materials with tunable multicolor emission on demand, especially for that in the solid-state. The current systems rely on the sophisticated synthesis of varied organic/polymeric fluorophores with different emission maxima, which often requires complex synthesis approaches with multiple steps and high costs. Recently, single organic fluorophore molecules were found to show multicolor or even white emission by changing the aggregate structures. This is achieved by varying the molecular packing through chemical modification, thermal treatment, or solvent exchange. However, this strategy requires precise engineering of the polymorphic state of the fluorophore molecules, which can be influenced by the environment during the manufacturing process. Therefore, robust multicolor emissive systems with simple chemical composition are still lacking. Here, a new strategy for the preparation of simple and tunable multicolor organic emissive systems was developed via aggregation-dependent single fluorophore molecule. A series of fluorescent polymers with varied molecular weight were synthesized by atom transfer radical polymerization. Their fluorescence properties were investigated in aggregated state including both in bulk and nanoparticles. The polymers exhibited strong aggregation-induced emission (AIE) and polymer chain length-dependent fluorescence color, via simple macromolecular engineering. This strategy enables the efficient modulation of the molecular fluorescence in solid state by simply varying the molecular weight of the fluorophore-polymer conjugates via controlled radical polymerization.

9:00am - 9:15am

Detection of small targets using heteroligand-functionalized plasmonic particles.

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Detecting small target biomolecules, chemicals, or ions is a challenge that requires unique solutions. Most sensing mechanisms especially that of label-free methods rely on minimum level of molecular size, which typically tens of kDa, exerting significant biophysical impact of its presence. Here we describe how the use of heteroligand, instead of the usual monoligand system in plasmonic-based detection can increase the efficiency of plasmon coupling (PC), and hence resulted in a better biosensing signal. PC optimally occurs when two plasmonic particles at the vicinity lower than 4 nm distance. This means target that has a diameter within that range is somewhat advantageous to be detected. However, two typical problems would arise; 1) the capturing agent (ligand or bioreceptor) usually dissipates the dynamic space of the detection, and 2) the target, which is usually chiral in nature, not optimally treated as such during the capturing event. Therefore, using a heteroligand system where different ligand is anchored onto different

nanoparticles, both setbacks will be minimized. This work will open new avenues for in-situ small pollutants, and metabolites detection that would benefit both environment and healthcare in the near future.

9:15am - 9:30am

Emerging Applications of Boron Nitride Nanotubes for Advanced Electronics and Bio-imaging

Yoke Khin Yap

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The electrically insulating and optically transparent boron nitride nanotubes (BNNTs) have found novel applications in advanced electronics and bio-imaging. Although these physical properties are not favorable for conventional electronics and energy applications, recent advancement in controlled synthesis of BNNTs has enabled the demonstration of a series of unique application. [1-3] For example, BNNTs are unique one-dimensional templates for room-temperature single-electron transistors (SETs) [4], two-dimensional gold quantum dots with tunable optical bandgap [5], field-effect transistors (FETs) by van der Waals atomic chains [6], and immunophenotyping by flow cytometry [7]. Details of all these emerging applications will be discussed in the meeting.

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9:30am - 9:45am

Magneto responsive surfaces for manipulation of light and liquids

Matija Lovšin¹, Gaia Kravanja², Inna Belyaeva³, Luka Hribar², Gašper Glavan³, Matija Jezeršek², Mikhail Shamonin³, Irena Drevensek-Olenik^{1,4}

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Magnetoactive elastomers (MAEs) are rubbery substances composed of a soft polymer matrix with embedded micrometer-sized ferromagnetic particles. They are also known as magnetorheological elastomers (MREs) and are often perceived as solid analogues to magnetorheological fluids. Hitherto, the majority of research on MAEs was concentrated on their bulk properties. However, recently it has been realized that surface properties of MAEs substantially alter in a magnetic field too, which opened a new emerging research field associated with them. The main underlying mechanism of magnetically tunable surface properties of MAEs are magnetic field-induced modifications of their surface roughness. Due to this property, MAEs are an excellent candidate for magneto responsive surface coatings with dynamically tunable characteristics. We investigated the effect of an external magnetic field on the splashing behavior of ethanol drops impacting on the surface of soft MAEs. The Weber number corresponding to the transition between the deposition and the splashing regime decreases with increasing magnetic field. Alongside this effect, a significant increase of the initial deceleration of the ejection sheet also takes place. We studied also the effect of magnetic field on reflection of laser light from a MAE surface. With increasing magnetic field, the specular reflection is transformed to spread reflection. Moreover, the total reflectivity from the surface is also strongly reduced.

Acknowledgements

Financial support of reciprocal visits by the Slovenian Research Agency (ARRS, project no. BI-DE/20-21-11) and the German Academic Exchange Service (project no. 57513473) in the framework of the project "Smart magneto-sensitive coatings for controllable droplet splashing" is gratefully acknowledged. We also acknowledge financial support by the ARRS in the framework of the research programs P1-0192-Ligh and Matter and P2-0392-Optodynamics.

9:45am - 10:00am Warning: This presentation lies outside the session time!

Neutron scattering on yttrium iron garnet under ultrasound injection

Shin-ichi Shamoto^{1,2,3,4}, Mitsuhiro Akatsu⁵, Masato Matsuura¹, Jun'ichi Ieda³

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In yttrium iron garnet YIG [1], the spin current has been observed as a spin Seebeck effect under a temperature gradient [2] and ultrasound injection [3,4]. The neutron scattering on a YIG single crystal under ultrasound injection has been performed by using DNA (BL02) with high energy resolution, to study the spin pumping effects on magnetic Bragg peak and magnon. At room temperature, a

magnetic Bragg peak at (220) was only slightly enhanced by the ultrasound injection, whereas the effect was significantly increased at low temperatures. The peak width in energy was also increased depending on the applied voltage at the LiNbO₃ transducer. In YIG, so far, an anisotropic magnetic capacitance effect is observed at low temperatures [5]. In this project, we accidentally discovered that the Zeeman energy gap diminished significantly at low temperatures only under a magnetic field along the [111] axis in the same temperature range [6,7]. Our recent result on Er₃Fe₅O₁₂ will also be presented. This anomaly was confirmed by specific heat and magnetization. The spin-lattice coupling will be discussed as to their possible origins of the anomalies. This work has been performed at DNA(BL02) of J-PARC MLF under the proposals 2017L0301, 2014B0157, 2015I0002, and 2016A0318.

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EPMM-INV-3: Electronic, Photonic and Magnetic Materials

Time: Friday, 20/Aug/2021: 10:20am - 12:30pm · Virtual location: AU 2410

Session Chair: Rainer Timm

10:20am - 10:35am

A non-trivial view of the metal-molecule electron transfer: Chemical, electrical and photonic factors

Samuel Valdivia, Daniel Aranda, Francisco J. Avila-Ferrer, Isabel López-Tocón, Juan Soto, Juan Carlos Otero

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This communication deals with the properties of molecules bonded to charged metal surfaces (electrodes, nanostructures or clusters), especially focused on the charge transfer (CT) process. The energy requirements for forward (F-CT: metal-to-molecule) and reverse (R-CT: molecule-to-metal) electron transfer are usually explained on the basis of very popular schemes based on the relative position of the Fermi level (FL) of the metal with respect to the energies of the LUMO (F-CT) or the HOMO (R-CT) orbitals of the molecule (Fig. 1). The electrode potential (EV) is a key parameter given that, for instance, negative shifts (-EV) raise FL and, therefore, reducing EF-CT and increasing ER-CT, respectively: $-eEV = EF-CT = ER-CT$.

In such scheme metal and molecule are not "connected", the only role of EV is to shift FL. Several photoelectrochemical experiments do not support this trivial energy conversion $G = ECT/EV = 1$ eV/V. Experimental G values are very scattered but shows unexpected huge energy gains ($G = 3-5$ eV/V [1]) which can be explained on the basis of theoretical calculations. DFT calculations on charged metal-molecule hybrids are able to explain the complex dependence of the properties of the interface on the chemical nature of their constituents and on the subtle effect of applied potentials giving huge [1] or zero energy gain [2], depending on the strength of the surface complex. The metal-molecule hybrid system has two different electronic structures which are selected by the sign of the surface excess of charge of the metal. Besides G values, this dual electronic structure shows a sharp change in other properties as the dependence of the adsorption energy or the vibrational wavenumbers on the applied voltage.

10:35am - 10:50am

Experimental Observation and Theoretical Modelling of Light Activated Resistance Switching in Single ZnO Nanowire

Justin Derickson Derickson¹, Kausiksankar Das¹, Benjamin Barnes²

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Semiconductor nanowires are the building blocks of many nanoscale electrical and neuromorphic circuits. Here, we demonstrate a simple arrangement wherein an ethanol-adsorbed ZnO single nanowire, deposited between gold electrodes using dielectrophoresis exhibits significant change in resistance when activated by visible light. We have observed that the transition timescale between two stable ohmic states, one in the dark and the other in the illuminated regime in a single nanowire can occur in the sub millisecond order, which is 7 orders of magnitude lower than previously reported switching timescale in bulk ZnO thin films. We also demonstrate that visible light acts as a non-invasive tuning parameter for the bistable resistive states that can be potentially used as memory switches in synaptic circuits. A mathematical model of the light activated resistance switching mechanism is proposed based on the adsorption-desorption kinetics of oxygen molecules at the surface of the nanowires, which shows promising agreement between theory and experimental results.

10:50am - 11:05am

Noninvasive analyses for brain disease by monitoring angle-coherent spectra from photonic quantum ring laser of whispering gallery modes

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Noninvasive diagnoses by angle-resolved coherent tomographic infrared spectroscopy (ACTIRS) are presented, where 3-dimensional (3D) angle-resolved light cones (ARLCs) from photonic quantum ring (PQR) laser of whispering gallery mode (WGM) are employed. It is important that we analyze the return spectra optically, not photocurrent-converted as for conventional FNIRS, after the cortical, vascular or muscular diffuse brain paths. The unique angle-coherent multi-spectra will eventually lead to ionic or protein analysis associated with cranial tissue or arterial line before that is obtained only from uncomfortable brain MRI, CT or biopsy.

PQR laser location (L) and the track of an angle(e.g., ~30°)-resolved light cone (ARLC) where (C)-fiber probe can be placed at a selected point for detecting return signals of specific blue-shifted wavelength. Then about 3 cm penetration depths (BIOPAC's FNIRS sys. estimates) let us imagine an equilateral triangle of L - C (fiber probe) - T (target region), being a cross-section of a schematic ARLC (Fig.1a), agrees and roughly follows the blue-shifted diffuse paths (~30° inclination); PQR's spectral paths through frontal lobe (red and) blue diffuse paths are consistent with blue-shifted incident laser as shown in Fig. 1b. The paths consisting of heterogeneous media in general will need further investigations.

The PQR laser, a cylindrical mesa structure of active Ga(Al)As or InGaAs multi-quantum well (MQW) plane between top and bottom DBRs, functions as concentric quantum-wire emitters within the PQR's peripheral Rayleigh band of 2-dimensional (2D) MQW circles, which is associated by nature with traditional 2D WGM phenomena in x-y plane as explained by Lord Rayleigh in 1912. The PQR Rayleigh band plane is optically surrounded by new 3D whispering cave mode (WCM) regions due to DBRs. The systematic variations of intermodal spacing agree with a well-defined angular quantization rule, while the VCSEL peak, λ_0 , shows no spectral profile (Fig. 1b).

Figure 1: (a) (b)

11:05am - 11:20am

Overview of spark plasma sintering of functional ceramics

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Abstract: The non-conventional Spark Plasma Sintering (SPS) process is based on the combination of a high current and a mechanical high pressure applied directly to the powder material. This technique presents the advantage to provide the possibility to obtain dense materials in a few minutes while mastering their microstructure. A lot of works have been reported since the introduction of SPS in research laboratories, and many groups have tried to understand the densification mechanisms involved.

After a brief history of the SPS technique, the characteristics of this process will be detailed and compared to those of the other sintering techniques.

On the other hand, the densification, the texturation and also the functional properties of materials sintered by SPS will be discussed. We'll successively consider: i) the sintering of recycled Nd₂Fe₁₄B magnets; ii) the fabrication of superconducting MgB₂ cryo-magnets and iii) the fabrication of layered superconducting Bi₂Sr₂Ca₂Cu₃O₁₀ bulks. In this last case, the SPS equipment was modified in order to obtain textured bulk samples. This new process is referred to as "Spark Plasma Texturing" (SPT). During SPT, the bulk material can freely deform. As a result, a preferential crystallographic orientation of the grains is obtained. The anisotropic properties resulting from the grain alignment will be discussed.

11:20am - 11:35am

Neural Probes and Through-Silicon-Via Interposers: Utilizing High Aspect Ratio Carbon Nanotube Arrays

Guohai Chen¹, Rajyashree Sundaram¹, Atsuko Sekiguchi¹, Robert C. Davis², Kenji Hata¹, Don N. Futaba¹

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Assembling nanomaterials into arbitrary architectures is vital step in defining their role in any application. Vertically aligned carbon nanotubes (VACNTs) represent an interesting multifunctional nanomaterial to construct larger macroscopic assemblies for applications. In this talk, I will present our work on the fabrication and utilization of VACNT pillars. First, I will discuss our approach to enable the fabrication of high aspect ratio (60:1) free-standing CNT pillars possessing high uniformity [1-3]. To maintain perfectly vertical growth of each pillar within the array of mm-tall, high aspect ratio VACNTs, "hedge" structures were employed as support but later removed. As a result, 1.2 mm-tall and 20 μ m-diameter pillars were achieved. Second, I will present two diverse applications utilizing two different aspects of this porous structure. In one case, we applied these high aspect ratio and mechanically compliant posts as microelectrodes as a candidate for neural probes. Examination of the electrochemical detection to methyl viologen and dopamine using an individual CNT microelectrode showed fast-electrochemical response. In another application, we demonstrate the feasibility of CNT-Cu as a via material for through-silicon-via (TSV) interposers which can potentially possess both high electrical conductivity of Cu and low coefficient of thermal expansion (CTE) of CNTs, after a two-stage Cu electrodeposition [4, 5]. The CNT-Cu TSV showed Cu-level electrical conductivity ($\sim 2.5 \times 10^5$ S/cm) and Si-level CTE ($\sim 7 \times 10^{-6}$ /K). The greatly reduced CTE mismatch between CNT-Cu and Si was achieved and its functionality was demonstrated.

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11:35am - 11:50am

Materials processes and characterization of rare earth doped layered ferroelectric ceramics for random access memory devices

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Modern computer systems employ the nonvolatile random access memory (NVRAM) device embedded in an integrated chip to store information. Ferroelectric random access memory has been utilized in NVRAM owing to its distinct properties such as low power consumption; fast read/write performance and high endurance compared to other electrically driven memory devices. Even though the classical ferroelectric lead zirconate titanate material has been extensively studied, practical application of this material is limited since it undergoes severe polarization fatigue during cyclic polarization switching and also this material is highly toxic. On the other hand, the renewed interest stems from the layered ferroelectric materials such as SrBi₂Ta₂O₉, SrBi₂Nb₂O₉, BaBi₂Nb₂O₉, Bi₄Ti₃O₁₂ due to the low fatigue with polarization switching and nontoxicity. However, these materials exhibit two significant drawbacks: High processing temperature and low remnant polarization. It is recently found that trivalent rare-earth ions doping on the crystal lattice of these layered ferroelectric materials significantly influence the physical properties. In our present research, the influence of samarium ion doping on the structural, microstructural, dielectric and electrical conductivity characteristics of SrBi₂Ta₂O₉ and BaBi₂Nb₂O₉ ferroelectric ceramics synthesized by molten salt synthesis route has been investigated in detail. The X-ray powder diffraction studies have revealed monophasic perovskite crystalline structure of different concentrations of samarium ion doped

ferroelectric ceramics. The existence of plate-shaped morphological features of these ceramics has been demonstrated through scanning electron microscopic studies. The dielectric and electrical conductivity characteristics on these ceramics have given unique insights into the structural - property correlations. This talk shall provide a brief overview of layered ferroelectric materials widely employed in random access memory devices and present our recent research on the influence of rare-earth ion doping on their physical properties.

11:50am - 12:05pm

Investigation of PMMA/C60 nanocomposites as nanophotonic materials for potential medical application

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Nanocomposites made of PMMA - Poly(methyl methacrylate) with different concentrations of fullerene C60 proved to have interesting optical properties and thus may serve as a good new material for spectacles. Because the structural properties of PMMA/C60 complex depend on the arrangement of methyl methacrylate (MMA) and C60 molecules, several nanocomposites (PMMA/C60) having different concentrations of fullerenes (0.025 wt.%, 0.05 wt.%, 0.075 wt.%, and 0.1 wt.%) were created and characterized by Magnetic Force Microscopy and UV-VIS spectroscopy. It is demonstrated that the structure of the complex directly correlates to the ratio of unpaired/paired electrons within the material. Also, Magnetic Force Microscopy was used to demonstrate the influence of different concentrations of fullerene molecules in PMMA on the attraction and the repulsion forces and consequently on the complex structural and optical properties. Based on investigation it is demonstrated that the PMMA/C60 complex with 0.025 wt.% concentration of C60 has the best structural and optical properties to be applied as a new material for spectacles. Based on UV-VIS Spectroscopic analysis in the domain of 380 to 780 nm this concentration reduces UV and high blue energy light by more than 60%. Further, spectroscopic analysis of the influence of diffuse and linearly polarized light was done in domain 200-1100 nm, while the influence of green and red light before and after the interaction was separately done. It is demonstrated that the total difference of 42.26%, between diffuse and linearly polarized light of the same source of light, before and after the interaction with C60/PMMA complex exists. Analyzed experimental data performed by scanning tunnelling microscopy, strongly indicating that during C60-light interaction, exciton, as quantum 0D cavity phenomenon, is created that makes strong coupling with photons, creating polaritons. The hyperpolarizability property of C60 and photon half-quantization of its optical angular momentum create a new type of illumination (sunflower shape). Based on obtain results, the initial ophthalmological study, based on 50 volunteers, in the field of contrast sensitivity was conducted, and obtained positive results indicate that more, both scientific and clinical medical investigation of C60-light interaction, are needed.

12:05pm - 12:20pm Warning: The presentations finish prior to the end of the session!

Electron-phonon coupling in semiconductor nanostructures: intrinsic and extrinsic tunability demonstrated with ZnTe nanowires

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The dependence of electron-phonon coupling (EPC) on nanostructure size has been a topic of controversial over three decades. Often, the EPC was probed by resonant Raman scattering (RRS) using the 2LO to 1LO intensity ratio R21 to extract the Huang-Rhys factor [1] (S) by applying Albrecht's theory,[2] where the bulk reference S was calculated by using a theoretical model developed for a bound exciton with Fröhlich interaction.[3] The issue involves multiple aspects: (1) What would be the appropriate mechanism for the nLO Raman lines in the bulk material, since they already exist in the bulk material and are only modified in the nanostructures? (2) What does R21 tell about EPC? (3) Were the observed changes of intrinsic to the nanostructures? We note that the S factor and Albrecht's theory both are based on lattice relaxation that typically occurs when a highly localized state is involved in an optical transition. Thus, they do not apply to the nLO in RRS in bulk and likely to most cases of the nanostructures.[4] Since R21 has been found to be very large (because 1LO is very weak) in high quality bulk materials, decrease in R21 actually implies increase in EPC for the specific process rather weakening in EPC as often suggested.[5] We have shown [6] that in ZnTe, in contrast to the previous reports, R21 exhibits a much larger intrinsic value and minimal change from bulk to 30 nm nanowire, indicating previously reported size dependences were likely affected by extrinsic mechanisms. In fact, the ratio can be tuned extrinsically over one order in magnitude controllably either during or post growth, allowing for programing EPC in nanoscale devices. Similar degree of tunability has also been demonstrated in ZnTe thin-film samples. This work provides unambiguous experimental results for developing EPC theories for reduced dimensionality and defect influence, and suggests the need to reexamine the reported results for different material systems to distinguish the intrinsic and extrinsic effects.

Key Words: Nanostructures, Electron-phonon Coupling, Resonant Raman Scattering

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FCM-INV-1: Functional Composite Materials

Time: Friday, 20/Aug/2021: 10:20am - 12:30pm · Virtual location: Theatre

Session Chair: Adam Weber

10:20am - 10:35am

Self Sensing Cement-based composites with Short Carbon Fibers

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This paper is aimed at exploring mechanical, electrical and self-sensing properties of cement-based mortars through the addition of short carbon fibers, at different dosages (2%, 3%, 4% by weight of cement). Compression and bending tests on carbon fiber reinforced cement-based materials (CFRCM) were performed. The addition of carbon fibers showed to enhance the mortars' flexural strength by increasing the fibers content, while no improvement was found in the compressive strength. Electrical resistivity of the CFRCM, at different days of curing, was evaluated by AC impedance measurements, using two stainless steel wire meshes as electrodes. The electrical resistivity decreased with time, until reaching a constant value after about 60 days of curing. Carbon fibers were able to drastically reduce the mortar resistivity, up to values below 150 Ω cm. The effect of fibers dosage on the ability of the mortar to change its electrical resistivity when subjected to different stress states was also studied. The specimens were gradually loaded up to 50–60% of the maximum compressive strength, carrying out two loading/unloading cycles, while resistivity was measured using a conductivity meter. Depending on the fibers dosage and stress state within the material, CFRCM resistivity changed with significant variations.

10:35am - 10:50am

First-Principles Calculations of the Energy Flux for Bioinspired Personalized Thermal Comfort Wearables

George T Stiubianu¹, Alexandra Bargan¹, Mihaela Dascalu¹, Carmen Racles¹, Adrian Bele¹, Codrin Tugui¹, Cristian Ursu², Maria Cazacu¹

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Thermal management is important for modern technologies - buildings, electronics, and clothing. The animal kingdom offers inspiration for development of materials with excellent thermal management, such as the mirror comb-footed spider (*Thwaitesia* sp.). The fast dynamic optical color changing capabilities of organelles found on the abdomen of this spider has provided inspiration for new polymer nanocomposite materials with application in thermal management. The developed materials replicate the capability of aforementioned spiders to change the reflectance and transmittance of light in the infrared wavelength range. The nanocomposite materials are safe for human use and are scalable for large-scale application.

The new polymer materials bring together the advantages of passive thermal control (low cost, easily scalable implementation, and efficiency in terms of on/off switching ratio), with on-demand control of temperature specific for active thermal control for unparalleled thermal management. The procedure (Figure 1) can be scaled up with well-known methods for polymer film formation. Our team used the versatile chemistry of silicone and styrene polymers for preparation of films that can manage up to 60 W/m². This capability for managing the thermal flux can be tuned in real time by mechanical or electrical actuation, with an input of <5 W/m². Inside office buildings ~60% of the heat exchange between the human body and the environment takes place through infrared radiation, and the nanocomposite materials in unactuated state can reflect infrared radiation as well as the space blanket developed by NASA in 1960. By mimicking the change in surface area of the plates on the spiders' abdomen, the nanocomposites can modulate up to 70% of the heat flux emitted by the human body. With introduction of such materials in clothing, the thermal comfort range can be expanded, leading to ~3% energy savings of global commercial energy consumption.

Acknowledgements: This work was supported by a grant of the Romanian Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-III-P2-2.1-PED-2019-1885, within PNCDI III (Contract 463PED/2020).

10:50am - 11:05am

High-performance silk-based bioplastic from regenerated fibroin

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Due to the unique combination of properties such as mechanical strength and toughness, biocompatibility, biodegradability, thermal stability, and easy processability [1,2], regenerated silk fibroin has been used as a functional biomaterial, adopted when a positive interaction with living tissue is required. While a plethora of micro and nanoscale architectures of silk fibroin have been explored in literature - films, fibers, microparticles, and gels, building - larger, macroscale objects of fibroin has been challenging.

In this work we report a method to obtain a compact material form fibroin powder in a single compression mold step. We were able to optimize a fast, low temperature method to obtain large monoliths of solid - fibroin, reporting, for the first time a thermal - reflow at 40 °C for lyophilized silk fibroin [3]. With this technique large objects can be produced in few minutes with a high reproducibility. The mild forming conditions allow the possibility to incorporate temperature degradable bioactive additives. The possibility of post sintering molding through CNC machining or laser cutting allow the easy realization of user-defined shapes, making this biodegradable material suitable for several applications, included the design of biomedical implantable devices.

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11:05am - 11:20am

Lifetime improvement of anticorrosive hybrid coatings by addition Li and Ce self-healing agents

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Organic-inorganic coatings based on polymethyl methacrylate (PMMA)-silica hybrids provide effective and active corrosion protection of metallic surfaces against corrosive species. The covalent conjugation on the molecular scale between and the PMMA matrix, provided by the propyltrimethoxysilane or 2-hydroxyethyl methacrylate coupling agent, leads to a homogenous and highly cross-linked nanocomposite, which in form of coatings act as an efficient diffusion barrier. Transmission electron microscopy, small-angle X-ray scattering, and thermal analysis data showed that the addition of increasing amounts of lithium carbonate or cerium ammonium nitrate (0, 500, 1000, 2000, and 5000 ppm) to the silica precursor solution (tetraethoxysilane - TEOS) yields PMMA-silica coatings with increased connectivity of the silica cross-link nodes, uniformly distributed in a highly polymerized PMMA matrix. Results of electrochemical impedance spectroscopy (EIS) assays of coated aluminum AA7075 aluminum alloy, performed in a 3.5% NaCl solution, showed that the addition of Li or Ce provides for both coating systems the self-healing ability resulting in a significantly improved lifetime up to 720 days and an impedance modulus of up to 50 GΩ cm². Time-of-flight secondary ion mass spectrometry, scanning electron microscopy and X-ray photoelectron spectroscopy suggest that the regeneration process occurs by leaching of lithium/cerium ions from the coating surface into the corroded area, which is restored by a protective layer of precipitated species.¹ An analog mechanism was found for artificially scratched coatings presenting an impedance modulus increase after neutral salt spray test compared to the bare aluminum alloy. These findings evidence the active role of lithium and cerium ions in improving the structural properties of hybrid coatings and providing through the self-healing ability a significantly extended service time of metallic components.

11:20am - 11:35am

Making stretchy dielectric, conductive, and semiconductor polymers

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The increasing demand for devices that are deformable, wearable, or implantable has been driving the development of functional materials that are additionally compliant and repeatedly stretchable. I will introduce our recent efforts in developing elastomeric dielectrics, semiconductors, and conductors. The formation of interpenetrating networks and other microstructural control techniques are used to (1) enhance the electromechanical responses of dielectric elastomers, (2) protect the conductive percolation network of silver nanowires and carbon nanotubes at large-strain deformations, and (3) to impart elastic deformability to semiconductor materials that are otherwise not stretchy. Explorations of devices incorporating these materials will also be presented.

11:35am - 11:50am

Microstructure evolution of silicon carbide reinforced PEEK under tribological solicitations

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Minimizing the environmental impact of human activities is a challenge going towards sustainable and efficient materials. New polymer matrix composite materials are elaborated for high-performance applications such as aerospace and aeronautics. We have developed innovating multifunctional composites with a polyetheretherketone (PEEK) matrix and silicon carbide (SiC) particles. Specimens are prepared with microparticles, or nanoparticles by melt-blending then shape by thermo-pressing.

While bringing higher mechanical strength, this process improved the tribological performances of our semicrystalline thermoplastic material.

Our research focused on microstructure changes under tribological strain in the PEEK matrix, and the effect of silicon carbide particles on this tribological behavior.

We have performed sliding tests with ball-on-plate configuration and reciprocating translation motion. The plastic deformation dominates the accommodation mechanisms, and the material loss is reduced with SiC addition. Moreover, our results highlight the microstructure changes of PEEK and the composites due to the tribological solicitations: with Raman spectroscopy, we have followed locally the crystallinity rate evolution in the wear track and depending on tribological tests duration. We conclude that the crystallinity rate decreases with the contact pressure and the tribological test timespan.

11:50am - 12:05pm

Developing Lightweight Homogeneously Mixed Heat- and Current-stable Cu/Carbon Nanotube Composite Electric Conductors

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We present our progress with developing homogeneously mixed copper-carbon nanotube composites (Cu/CNT) lighter than copper with rivaling electrical conductivities as well as heat and current-stabilities. Such materials are expected to function as more durable



lightweight copper-alternatives in aircraft/automobile electrical wirings for improved weight-reduction and fuel-efficiencies as well as in micro-interconnects for smaller more powerful electronics [1]. To demonstrate macro and microscale applicability, we fabricated Cu/CNT with excellent performances in a variety of structures including cm-scale wires and microscale via-like structures by Cu-electrodeposition of CNT templates [2-6]. Irrespective of structure, our composites show densities $<5.2 \text{ g/cm}^3$ and are at least 2/3rd as light as copper. Such low densities could be achieved by tuning composite fabrication to incorporate high nanotube vol% ($>40\%$) with homogeneous CNT-Cu mixing. Room temperature electrical conductivities of our lightweight Cu/CNT are $\sim 1-4 \times 10^5 \text{ S/cm}$ competitive to that of pure copper ($5.9 \times 10^5 \text{ S/cm}$). The temperature stable conductivity of our composites is reflected by temperature coefficients of resistivity (TCR) as low as 10% that of copper. In terms of current stability, our Cu/CNT's current carrying capacities (CCC) surpass that of copper. Our composites also show better thermal expansion stability with coefficients of thermal expansion (CTE) $\sim 4-7 \text{ ppm/K}$, closer to Si-CTE ($\sim 3 \text{ ppm/K}$) than Cu-CTE ($\sim 17 \text{ ppm/K}$). Besides demonstrating Cu/CNT's promise as a Cu-substitute, we will discuss the various factors (Cu and nanotube spatial distribution, nanotube attributes, metal/nanotube interface, etc.) that affect composite properties to provide pointers for Cu/CNT performance tailoring.

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12:05pm - 12:20pm

Bio-factory mediated and biomimetic approaches for the synthesis of SiO₂- based nanostructures for multiple applications.

Alessandra Aloisi¹, Riccardo Di Corato¹, Gianluca Farinola², Paola Nieri³, Rosaria Rinaldi^{1,4}

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A novel biotechnological approach to the preparation of Ir-doped luminescent silica-based nanostructures is proposed availing use of diatoms microalgae which generate highly nanostructured biosilica shells (frustules) by in vivo biomineralization of orthosilicic acid [1]. After the in vivo incorporation of a phosphorescent organometallic complex (Ir-1) in *Thalassiosira weissflogii* diatom frustules (DFs), bulk functionalized phosphorescent silica-based nanostructures are obtained by isolation and proper ultrafine processing of Ir-1-doped DFs. High-resolution characterization reveals the presence of phosphorescent hybrid organic/inorganic clusters composed of biogenic silica NPs intimately trapped within the diatom organic residual matter. The biofactory strategy investigated herein can be a sustainable, cost-effective, and scalable route to transition metal-doped silica nanomaterials and can pave the way to a great variety of heavy-metal and rare-earth metal doped silica nanostructures, whose applications range from photonics to imaging, sensing, and biomedicine.

Inspired by the biosilica morphogenesis, which takes place inside the diatom cell within the silica deposition vesicle (SDV), a specialized membrane-bound compartment, we set up a biomimetic/bioinspired design and synthesis of structural and functional hybrid organic/inorganic SiO₂-based nanostructures (NSs), which present many distinctive advantages over traditional chemical synthesis methods. The intriguing ability of diatom long chain polyamines (LCPAs) to rapidly induce precipitation of SiO₂ spheres has motivated the in vitro one-pot synthesis of SiO₂ particles. Therefore, the templating by amine-bearing molecules is seen as a successful biomimetic approach for the synthesis of SiO₂-based hybrids under mild and environmentally friendly conditions for biosensing and biomedical applications. [2].

Key Words: Biosilica; Nanoparticles; Nanostructures; Microbioreactors

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12:20pm - 12:35pm Warning: This presentation lies outside the session time!

GFRP Full Adhesive Connections: Mechanical Aspects

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In the field of the fiber reinforced polymer materials the efficiency of the adhesive technique versus the classical ones, bolting and welding, has been demonstrated by several studies available in the literature [1,2]. The main advantage of adhesive technique is relative to the absence of holes, then the stresses are more uniformly distributed over the bonded surfaces and stress concentration and damage to the fibers caused by the holes are non-existent. Furthermore, the stiffness and strength of adhesive joints is generally sensibly higher than those of bolted connections [3]. On the contrary, full adhesive joints present a brittle unsolicited behavior as well as an innate absence of plasticity limiting the diffusion on this technique in the field of civil engineering in particular. Within this

framework several studies were developed to the study of hybrid connection (bonded and bolted at the same time), using the stiffness of the adhesive and the plasticity of steel bolts [4-5]. The main conclusion of these studies is that the strength of the hybrid connection is strictly function of the adhesive layer while the steel bolts represent a plastic reserve.

Relative to the field of full adhesive connection between FRPs members, in the present paper a wide experimental study is presented concerning the study of the mechanical response of a beam-to-column connection. Several parameters were taken into account: the extension of the adhesive surface, the load condition (shear and shear with bending) and the contribution of the GFRP angles. The test set-up was equipped not only with several displacement transducers in order to evaluate the load-displacement and moment-rotation curves but with the Digital Image Correlation system also. The latter allowed to understand the strain/stress distribution inside the adhesive layers giving the possibility to govern the strength and stiffness of the beam-to-column connection in function of the mode II of fracture energy being the only fracture energy considered. Furthermore, two different levels of fracture energy were taken into account: the total fracture energy, corresponding to the complete collapse of the joint; and the fracture energy level corresponding only to the linear behaviour of the connection.

FCM-INV-2: Functional Composite Materials

Time: Friday, 20/Aug/2021: 10:20am - 12:30pm · Virtual location: AU 2412

Session Chair: Alexander Ayzner

10:20am - 10:35am

Multi-Scale Materials by Effective Assembly of 1D and 2D Nanomaterials

Fabian Schuett¹, Florian Rasch¹, Lena Marie Saure¹, Armin Reimers¹, Ali Shaygan Nia², Yogendra Kumar Mishra³, Xinliang Feng², Rainer Adelung¹

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The fabrication of macroscopic and multi-scaled assemblies (such as sponges, foams, aerogels, etc.) from Graphene and related 1D and 2D nanomaterials is an extensively studied field due to their broad range of applications, such as in electronics, energy storage, catalysis as well as environmental protection. However, transferring the nanoscopic functionality of these unique materials into the macroscopic world is still challenging to achieve. In the here presented study, we demonstrate the versatile fabrication of multi-scaled framework architectures, composed of 1D and 2D nanomaterials, such as Graphene [1], hexagonal boron nitride (h-BN) [2], MXenes and carbon nanotubes [3]. With porosities in the order of 99.99% and densities as low as 0.2 mg/cm³ the properties of these so-called aeromaterials are determined by the nanoscopic functionality of the source material, enabling new applications. We demonstrate, that a multi-scaled material system composed of interconnected hollow h-BN microtubes, with a wall thickness well-below 25 nm, enables a novel class of high-brightness and efficient laser-based light sources. [2] The as-synthesized foam-like material forms a disordered and non-absorbing photonic network with thinly spread Rayleigh-type scattering centers, enabling a high degree in multiple light scattering. [4] Last but not least, we demonstrate that by exploiting the extreme low heat capacity of graphene-based aeromaterials cm³-sized gas volumes can be repeatedly and rapidly heated with heating rates beyond 300000 K/s and repetition rates of ~10 Hz. These "electrically powered explosions" demonstrate a reversible and environmentally friendly alternative to conventional chemical explosions, beneficial for applications in the areas of microfluidics, pneumatics, soft-robotics, propulsion systems, and thermoacoustics.

10:35am - 10:50am

Pathway to "Intelligence": Using Stimuli-Responsive Materials for Constructing Self-powered Autonomous Functional Systems

Siowling Soh

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Intelligent systems are characterized by their ability to sense their environments, analyze surrounding signals, and provide a logical response. Intelligence is exhibited in many complex biological systems (e.g., human beings and animals) and electronic-based machines (i.e., artificial intelligence). On the other hand, materials (e.g., bricks) are generally regarded as static, passive, and far from being considered as "intelligent".

This presentation discusses the approach of using stimuli-responsive materials as basic building blocks for constructing self-powered autonomous "intelligent" systems. "Intelligent" systems usually consist of a combination of functions: the analytical processing functions, regulatory functions, and practical functions for responding to their surroundings. Stimuli-responsive materials are used to construct these types of stimuli-responsive functions via the combination of smart composites, physical-chemical phenomena, reaction, and design. For the stimuli-responsive analytical processing functions, we showed that the combination of a stimuli-responsive hydrogel and an asymmetric unsteady-state reaction-diffusion process allows the material to perform calculus: the temporal derivative of concentration of the medium. Hence, we showed that materials with simple designs can directly perform advanced mathematical functions. We further showed that assemblies of stimuli-responsive hydrogels with simple designs can perform the functions of multiple logic gates for integrated circuits. For stimuli-responsive regulatory functions, stimuli-responsive hydrogels are designed to perform the functions of gating and self-amplification. For stimuli-responsive practical functions, stimuli-responsive hydrogels are found to produce large amounts of force onto their surroundings. Despite being soft materials, these stimuli-responsive hydrogels are able to grip onto loads that are ~10,000 times more than their own weights. By functionalizing the surface of the stimuli-responsive hydrogels, they are shown to be able to target, capture, and rupture cancer cells. Self-powered autonomous "intelligent" systems can thus be created by combining the different types of specifically designed stimuli-responsive functions for carrying out complex analyses and operations for a wide range of applications.

References:

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10:50am - 11:05am

Superantietting Polymeric Nanocomposite Materials: From Coating to Bulk Material

Stefan Seeger, Shanjie Liu, Georg Artus, Xiaotian Zhang

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Wetting and antiwetting is an important property of solid materials no matter if it is required or annoying. Several technologies have been reported to prevent wetting by water, oil, or even both. A major contribution was the development of silicone nanofilaments (SNFs) leading to extreme antiwetting coatings and meanwhile used in the industrial world. SNF technology is based on the new

Droplet Assisted Growth and Shaping (DAGS) synthesis approach where the formation of water nanodroplets is the key step for defining the shape of nanostructures finally providing superantwetting properties to a surface. Beside this, we will demonstrate a further step, how these materials can be further improved by nanocomposite approaches and we will introduce a tremendous step forward to stable superhydrophobic bulk polymer materials which do not suffer from the vulnerability of coatings. We will show a fluorine-free superhydrophobic bulk material with mechanochemical robustness and self-cleaning functionality based on polypropylene (PP) that simultaneously possess mechanochemical robustness and good resistance to oil fouling.

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11:05am - 11:20am

Effects of silica rich biochar on cement mortar hydration kinetics and durability under chloride and sulfate environment

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This study investigated influence of biochar, prepared from rice husk and waste wood, on hydration kinetics and resistance to chloride and sulfate attack of cementitious composite.

The resistance in terms of strength retention, mass change, expansion and micro-structural changes was studied and compared to similar properties of mortar under normal wet curing.

Findings suggest that rice husk biochar (RHB) contain 15–16% amorphous silica, although its carbon content (42%) and specific surface area are significantly lower than wood biochar (79% carbon and surface area of 227 m²/g). Both types of biochar at 1 wt% dosage increase rate of hydration at early stage than control, attributed to high surface area, finer size than cement and nucleation of cement hydrates on biochar surface. Both RHB and MWBC at 1–2 wt% significantly reduce water permeability than control, which is also reflected in 15–18% improvement in strength at 7-day, 42-day and 120-day age of cement mortar. Lower permeability due to addition of both biochar types reduces rate of mass gain due to sodium chloride absorption, contributing to 9% higher strength than control after 120-day exposure period. Based on strength, water-cement ratio and cement content, the tested mortars are suitable for exposure class of XS2 (EN 206), where the concrete is always submerged in water. When exposed to sodium sulfate solution, 1 wt% of RHB and 1 wt% of MWBC are found to improve strength by 14–17 % than control after 120-day, while minimizing loss in strength due to sulfate attack. Micro-structural analysis shows pore blocking action of biochar mitigates micro-structural damage due to sulfate attack. This offer higher dimensional stability, reflected from 62 to 68% less expansion of MWBC-mortar and RHB-mortar compared to control. These findings suggest suitability of biochar-mortar application under moderate sulfate environment.

11:20am - 11:35am

Dynamic Materials Inspired by Cephalopods

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Cephalopods (e.g., squids, octopuses, and cuttlefish) have captivated the imagination of both the general public and scientists alike due to their sophisticated nervous systems, complex behavioral patterns, and visually stunning camouflage displays. Given their unique capabilities and characteristics, it is not surprising that these marine invertebrates have emerged as exciting models for novel adaptive optical and photonic materials. Within this context, our laboratory has developed various cephalopod-derived and cephalopod-inspired systems with tunable functionalities within the visible and infrared regions of the electromagnetic spectrum. Our findings hold implications for next-generation adaptive camouflage devices and energy conservation technologies.

11:35am - 11:50am

High frequency operating shape changing resonators utilizing unique properties of SMA elements for (micro)robotics

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The magnetic field-driven (micro)robots are capable to deliver, manipulate and modify various micro-/nanoscale objects; therefore, they hold promises for either the controlled drug delivery to a specific area in human body or the non-invasive diagnosis and treatment. Currently develop magnetic field-driven robots transform the electrical energy into the mechanical work through a generated magnetic torque and/or force. However, strength of the magnetic field that drastically decreases with the distance from its source, complicates the necessary magnetic control and, consequently, restrict the widespread of these magnetic field driven (micro)robots. We report on an alternative contactless resonating architecture consisting of the polymer matrix embedded with NiMn₂Ga and NiTi elements. This actuation principle utilizes the anomalous softening / hardening in NiMn₂Ga caused by the magnetoelastic coupling and a low



magnetic anisotropy in its austenite phase, and the intentionally changeable prestress forces generated by NiTi elements. When NiMn₂Ga elements are subjected to prestress, the interplay between changes in the elastic properties of NiMn₂Ga during magnetization / demagnetization and the variable prestress originating from phase transformation in NiTi enables high frequency actuation and precise control of the bending of designed structure. We develop theoretical procedure capable predicting the behavior of these vibrating structures. Due to its relevance to actuation of micro-robots, we perform detailed analysis on multiple promising swimming mechanisms. The proposed architecture paves a way for further design of micro-(bio-)robots and contactless high frequency actuators and sensors with intentionally changeable shapes.

11:50am - 12:05pm

Self-adjusting boron nitride mask for Reactive-Ion Etching

Konrad Schwanitz, Marco Langenschwarz, Otto Fricke, Lorenz Kehrer

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In this paper a simple approach is demonstrated for spatially selective etching of a silicon nitride layer by Reactive Ion Etching (RIE) by using a reusable shadow mask as a separate solid component part. Two ceramics were compared as mask materials: aluminum oxide and boron nitride. After the usage of an aluminum oxide mask several times, the deposition of small aluminum fluoride particles is observed. In contrast, using a boron nitride mask, a RIE process without any residuals on the surface can be accomplished. Furthermore, cutting a shadow mask out of bulk material, containing a three dimensional structure, is feasible.

12:05pm - 12:20pm

Fine control of detonation nanodiamond surface chemistry towards functional materials

Hugues Girard

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Nanodiamonds (NDs) behave suitable chemical and physical properties for a wide range of applications in medical, energy or quantum domains. Detonation synthesis provides a mass production technique of well-controlled NDs, with a primary size of ca. 5 nm. However, a shell made of various surface terminations as well as graphitic or disordered carbon surrounds the diamond-core after the synthesis. The fine control of this superficial chemistry is essential to understand and take advantage of the interfacial and semi-conducting properties of NDs. For instance, a hydrogenated surface provides a negative electron affinity to the nanodiamond, which is deeply investigated to use them as a solid source of solvated electrons in water. On the opposite, an oxidized surface promotes the colloidal stability of NDs in different polar solvents, which is of great interest for the synthesis of nanocomposite.

This contribution will focus on the studies conducted in our group to better control NDs surface chemistries using thermal and microwave plasma treatments. The complementary combination of characterization techniques we used all over the years will be presented. Then, we will describe some applications in which surface chemistry plays a crucial role and directly drive the behavior of our nanomaterial, such as its incorporation in polymeric composite.

12:20pm - 12:35pm Warning: This presentation lies outside the session time!

Electric conductivity of CdSeZnS quantum dots dispersed in liquid crystals.

Cristina Cirtoaje, Emil Petrescu, Alina Petrescu-Nita

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Liquid crystals (LC) are continuous, organized and flexible structures that can host a large variety of particles. The smallest particles known so far, nanoparticles, are quite interesting for many applications so a deep understanding is needed to use them efficiently.

Unlike isotropic dispersions, liquid crystals allow us to obtain a reproducible structures that can be controlled by a external fields and provide valuable information about the electric or magnetic properties of inserted nanoparticles. A key point in this process is to identify and describe the interaction forces between the surface of the particle and the surrounding molecules. So far, we developed theoretical models and experimental studies [1], [2] for the electric response (i. e. Fredericksz transition) and dynamic behavior (relaxation times) of liquid crystal composite with quantum dots. This research helped us to understand the electric conduction process in liquid crystal cells with small amount of CdSe/ZnS quantum dots. By adjusting the quantum dots concentration, temperature and applied voltage and after comparing the results with theoretical

expectation, we obtained the electric parameters of quantum dots but also provided a procedure that can be used for other similar mixtures and particles. The may help the development of high performance electro-optic devices and improve the impact of technologies in research, industry and everyday life.

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Post-3: Poster Session

Time: Friday, 20/Aug/2021: 1:00pm - 3:00pm · Virtual location: Theatre
Session Chair: Umapada Pal

1:00pm - 1:03pm

Nonlinear optical organic-inorganic nano-composite DAST/AAO

Akshay Nagar, Peter Moroshkin, Jin Ho Kim, Jimmy Xu

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The organic salt 4-N,N-dimethylamino-4'-N'-methylstilbazolium tosylate, commonly known as DAST, has long been studied for its extraordinary nonlinear optical (NLO) properties [1]. In the bulk crystal form, it exhibits a high second-order nonlinear susceptibility $\chi^{(2)}$ that far outstrips that of many standard inorganic nonlinear crystals. This remarkable property of DAST has been widely exploited for THz generation, and recently further developed for second harmonic generation (SHG) in thin film forms, with results standing out in competition with even some of the best inorganic NLO crystals [2].

More recent experimental findings hint at the prospects of molecular engineering at the meso- or nano-scale for dramatically enhancing the nonlinearity via bond deformation.

Here we present a new series of further experimental investigations of the DAST molecular-engineering potential for enhancing its NLO properties through insertion of DAST into the nanopores of AAO thereby forming a novel organic-inorganic nano-composite. Underlying the heterogeneous incorporation is the creation of an intriguing interplay between a cylindrical stress built-in by Laplace's force that is inversely proportional to the diameter, the anisotropic ionic DAST, and an optical density of states and mode volume modified from that of bulk DAST by the local nanostructure.

The host AAO matrix is the anodized aluminum oxide (AAO) with nanometer-sized cylindrical pores perforating through the membrane. The DAST-AAO nano-composite films are subjected to 1064 nm nanosecond laser pulses and the SHG signal is measured as a means of assessing the molecular and nano-engineering effects on the NLO properties of the DAST. The SHG measurement was conducted in the reflection mode, necessitated by the sample inhomogeneity. Clear and substantial enhancements of SHG were observed in correlation with thermal annealing, attributable to recrystallization and bond deformation induced by the built-in stress and corroborated by additional tests under externally applied stress (by bending the films under test).

Acknowledgement: We are thankful to the support of AFOSR FA9550-19-1-0355 and ARO W911NF1420075; and to the DAST molecules synthesized and provided by Prof. X.D. Xu's group.

References

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1:03pm - 1:06pm

Novel exploitation protocols for capacitor lifetime enhancement

Justyna Piwek, Anetta Platek-Mielczarek, Elzbieta Frackowiak, Krzysztof Fic

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Sustainable energy storage devices like aqueous-based electrochemical capacitors (ECs) are intensively sought to ensure the novel technologies are clean, eco-friendly and cost-effective. However, water-based systems have not been successfully commercialized so far, while organic-based devices are already available on the market. To diminish negative aspects of strongly acidic or alkaline electrolytes (corrosion, safety), pH-neutral electrolytic solutions have been proposed; their environmental aspect and high hydrogen and oxygen evolution overpotentials allow the capacitor voltage to be exceeded far above theoretical water splitting (1.23 V). Lithium nitrate (LiNO₃) aqueous solution was proposed as a promising candidate for electrolyte in carbon-carbon symmetrical ECs. In one of our previous studies, the electrochemical performance of capacitors operating with 1 mol L⁻¹ LiNO₃ aqueous solution was investigated upon different voltage loadings (from 1.3 up to 2.0 V), and the origin of system fade (C/C₀=80% and ESR increase by 100%) was determined [1]. Mostly, two aging mechanisms were discussed accordingly to the voltage applied, with a value of 1.5 V as a discriminant between them. Positive electrode has been oxidized, and a deposit (e.g., Li₂CO₃) has been found on both electrodes after long-term floating tests. Nonetheless, the specific surface area (SSA) of the negative electrode is not remarkably affected by the aging process; the electrochemical hydrogen sorption is assumed to etch the electrode surface that might help to maintain high SSA, despite Li₂CO₃ precipitation.

In our next-step study, we propose advanced floating protocols as an alternative way for LiNO₃-based capacitor lifetime enhancement. Two optimization pathways are proposed (alternate and reversed floating) to exploit both electrodes' features fully.

This approach has been verified using different nitrate concentrations: 0.2, 0.5, 1 and 5 mol L⁻¹. Successful lifetime enhancement was achieved, up to +83% time prolongation (210 vs. 384 h of EC floating test with 0.2 mol L⁻¹ LiNO₃).

Acknowledgements: Authors acknowledge the European Commission and the European Research Council for financial support by the Starting Grant project (GA 759603) under the European Union's Horizon 2020 Research and Innovation Programme.

1:06pm - 1:09pm

On a Novel Magnetoelectric Oxide Cu₄O₃

Danijel Djurek¹, Aleksandar Živković², Nora H. de Leeuw², Mladen Prester³, Djuro Drobac³, Vilko Mandić⁴, Mile Ivanda⁵, Tatjana Jurkin⁵, Angela Pustak⁵, Danijela Bakarić⁵

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A laboratory preparation of paramelaconite (Cu₄O₃), a member of the group of natural minerals even more rare than diamond, is anything but a straightforward task[1]. In this work, a Cu₄O₃ phase stable up to, at least, 923 K was prepared via reduction of a cupric-copper oxide CuO. XRD and magnetic data agree well with those reported on the mineral sample[2], while magnetic susceptibility reveals an antiferromagnetic transition at 44,7 K. In contrast to other magnetoelectric materials, Cu₄O₃ exhibits a comparatively high electric conductivity 'sigma' = 110 S at room temperature (RT), most likely on behalf of the mixed valence structure Cu₂+Cu₂₂+O₃. Electric conductivity was shown to depend on frequency, and yields a strong resonance feature at 46,4 kHz at RT. From electric conductivity and time relaxation measurements one can calculate a magnetic permittivity $\mu_r = 2370$ and dielectric permittivity 'epsilon'_r = 6,6 · 10⁶. Calculation of electronic densities of states (DOS) provides the route to the Jahn-Teller (JT) distortion, as a precondition for the stress exerted onto the crystal lattice. Similar to other strong dielectric materials, a solely microscopic approach to the problem does not explain the huge dielectric permittivity. Here, we employ a Maxwell-Wagner (MW) model which is based on the mesoscopic properties and put forward an effect referred to the literature as internal grain boundary barrier layer capacitance (IBLC). In this work the IBL model was supplemented by a viscoelastic contribution on the grain boundaries, and use of the Maxwell-Voigt (MV) dashpot relaxation technique results in a Stieltjes-Riemann (SR) relaxation integral, while an application of the Lebesgue integration to SR gives back an extended form of the MW equation.

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1:09pm - 1:12pm

Preclinical Efficacy of MECA79-anti-CD3-Nanoparticles in Reversing Type 1 Diabetes

Ousama Rachid¹, Yousef Haik², Reza Abdi³

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Nanoparticles (NPs) have emerged as highly innovative materials to targeted delivery. Targeted drug carriers using polymeric-NPs hold particular promise to enhance the delivery of immunoregulatory agents to treat Type 1 Diabetes (T1D). We have recently formulated anti-CD3 loaded MECA-NP (MECA79-anti-CD3-NP) and showed their utility in prolonging heart allograft survival. We showed a significant increase in the T reg population in the draining lymph node (DLN) of MECA79-anti-CD3-NP treated transplanted animals and increased delivery to the DLN. We also fully characterized the fragments of MECA79 mAb following the reduction assay using TCEP, which shows mostly monomeric antibody. The average diameter of NPs was determined using dynamic light scattering to be 80.9±2.88 nm and 123.7±8.3 nm prior to MECA79 mAb conjugation and post-conjugation, respectively (p<0.01, n=3/group). To validate controlled release of anti-CD3 Ab from NPs, we studied the release profile of anti-CD3 up to two weeks in vitro. The results confirmed the gradual release profile of the anti-CD3 over time. Use of organic solvents during the NP fabrication step may affect the function of the antibodies. We then tested the preclinical efficacy of MECA79-anti-CD3-NP in reversing hyperglycemia in NOD mice (n=9 mice). Treatment was started at second consecutive day of blood glucose >250 mg/dL with i.v. administration of MECA79-anti-CD3-NP for five consecutive days followed by once a week treatment for 3 more weeks (n=7) (5 µg of anti-CD3/day/mouse). Amongst the 9 treated mice with MECA79-anti-CD3-NP, 7 mice responded to the treatment within a week (~78% acute remission rate) vs. 37% for the free anti-CD3 group (3 out of 8 mice). Free disease rate at day 45 (long-term remission rate was 75% for the MECA79-anti-CD3-NP and 40% for free anti-CD3 group. NO remission was noted in the untreated group (Figure 1). These data show a significant increase in therapeutic efficacy of anti-CD3 when it is delivered in the format of MECA79-anti-CD3-NP. It should be noted that these data for the first time showing the targeted delivery and superior efficacy using targeted nanoparticles in T1D. We sacrificed 2 normoglycemic NOD mice treated with MECA79-anti-CD3-NP. In contrast to the hyperglycemic NOD with no viable islets, there were viable insulin stained islets with T cell infiltrates around the islets (Figure 2).

Acknowledgements: "This work was made possible by the National Priorities Research Program award [NPRP9-350-3-074] from the Qatar National Research Fund (a member of The Qatar Foundation). The contents herein are solely the responsibility of the author."

1:12pm - 1:15pm

Production of Green Cementitious Composites: Granite Powder Utilization

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Nowadays, CO₂ emissions to the atmosphere have been growing steadily for several decades. Environmental protection has become one of the priority tasks of scientists from around the world. Researchers are trying to find ways to produce the most important materials that way, to reduce CO₂ emissions to the atmosphere. Cement is one of them. Cement production is one of the most adverse CO₂ emissions in the world (ca. 8% CO₂ emission in the world). Looking for opportunities to improve the natural environment, we should look for alternative material solutions (for example marble and limestone powders). Now, researchers are trying to reduce the amount of cement in cementitious mixes by replacing it with supplementary cementitious materials (SCM's). One of the most commonly used SCM in cementitious mixes are mineral powders (f.e. granite powder waste).

Granite powder waste is a waste material generated by crushing granite rocks or cutting granite rocks. So far, that material has been treated as waste, but the search for new SCM's caused, that it is increasingly used to reduce the amount of cement in cementitious mixes.

The main aim of the article is to determine the possibility of reducing the environmental footprint of cementitious composites produced with the use of granite powder waste. Comparative research were carried out related to the subject of fresh and hardened properties of cement mortars with the addition of granite powder waste. Based on the performed research, the main properties related to the utilization of GP in cement mortars are described. Additionally, the problems related to the preparation of this waste for use in the production of cements and cement mixtures were described. In order to determine the possibility of using granite powder waste in cementitious mixes, the results of the research carried out by the author and the results of other authors available in the literature were compared. The summary indicates the possible use of this waste to sustainable production of building materials.

1:15pm - 1:18pm

Self-adaptive radiative thermostat to surrounding temperature variation

Se-Yeon Heo, Gil Ju Lee, Do Hyeon Kim, Young Min Song

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Human beings use tremendous energy to keep cool in summer—current effective cooling, e.g., vapor compression and fluid cooled system consumes around 10% of worldwide energy [1]. This high level of energy consumption accompanies with various problems such as ozone depletion and greenhouse effect. To reduce the environmental burden on Earth, passive radiative cooling method is in the limelight in its eco-friendly way of lowering the temperature. However, it is unconscious and sustainable method lasts in winter and causes unwanted cooling. Although few prior studies reported efficient thermoregulation techniques [2,3], most of them uses additional energy or stimulation to change heating and cooling states. Here, we suggest surrounding temperature variant radiative thermostat (STVRT) to realize completely passive way for winter heating and summer cooling. The STVRT changes its cooling and heating states depends on designated temperature points. Our design consists of two core parts: partial solar absorber and thermal radiator within long-wavelength infrared region (LWIR) atmospheric window (i.e., 8-13 μm).

The appropriate solar absorbing portion is strongly needed to achieve winter heating. Based on thermal equilibrium equation, we extort the combination of $\sim 14\%$ of solar absorption layer (0.25-2.5 μm -wavelength) with $\sim 85\%$ of heat radiation layer (8-13 μm -wavelength). The proposed STVRT can reach $+9.6^\circ\text{C}$ heating and -7.4°C of cooling when surrounding temperatures are 0 and 30°C in ideal case (i.e., non-radiative heat exchange coefficient, $h_c = 0 \text{ W/m}^2/\text{K}$), respectively. For considering practical case, where $h_c = 10 \text{ W/m}^2/\text{K}$, the archived heating temperature is -2.2°C and cooling temperature is $+2^\circ\text{C}$ when surrounding temperature is 30 and 0°C , respectively. With these intuitive design, we experimentally demonstrate STVRT by coating using porous poly(methyl-methacrylate) (PMMA) (i.e., radiative layer) on Cu film (i.e., absorbing layer). The coating thickness of porous PMMA controls the solar transparency. Also, the material selection can be expanded as long as each layer takes engineered portion of absorption/emission. The design basic shows generalized solution for temperature homeostasis.

1:18pm - 1:21pm

Sintering mechanisms of core@shell metal@metal-oxide nanoparticles

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Metal@metal-oxide core@shell nanoparticles (NPs) have recently attracted increasing attention and show great potential for various applications, such as sensing¹, photo-catalysis², and dye-sensitized solar cells³. One prevalent phenomenon involving NPs in various applications is sintering (or coalescence), and it can be advantageous, or undesired. Sintering of NPs has been extensively studied using various computational methods, such as molecular dynamics (MD), investigating sintering of metals, metal-oxides, and bimetallic core@shell NPs. It is generally agreed that the dominating sintering mechanisms are surface diffusion and grain boundary diffusion in crystalline materials⁴ and viscous flow in amorphous clusters⁵. However, despite the fast-growing interest, no MD studies of the sintering mechanisms of metal@metal-oxide core@shell NPs have been reporting to date. Here, we present the atomic diffusion behaviours and sintering dynamics of three types of metal@metal-oxide NPs with crystalline metal cores and amorphous oxide shells that are investigated using molecular dynamics based on the ReaxFF potentials. The results show that the coalescence process is similar to reported mechanisms for crystalline nanoparticles. However, atomic trajectory tracing reveals that surface diffusion is highly localized and that it is mostly the surface atoms near the contact region that actively participate in the sintering. In other words, contrary to the common understanding of freely moving high mobility surface atoms, atoms located away from the contact region remain distant during the sintering.[1] We expect the sintering mechanism observed in metal@metal-oxide core@shell NPs here to be highly relevant for small metal nanoclusters as they usually have a thin surface oxide layer.

[1] N. Eom, M. E. Messing, J. Johansson, K. Deppert, Sintering Mechanism of Core@Shell Metal@Metal Oxide Nanoparticles, J. Phys. Chem. C, (2021), 125, 16220-16227

1:21pm - 1:24pm

Study of Hybrid Infrared Detectors with Perovskite Films and Quantum Dots

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The material class of perovskites has become a rising star in the optoelectronic applications. Over the very recent years it has demonstrated an astonishing growth of the power-conversion-efficiency in perovskite solar cells (more than 20%). Besides solar cells, perovskite photodetectors also achieved eye-catching results in the past five years. In the case of the visible light great detectivity, microwatt/mm² illumination level detection, and nanosecond response speed have already been achieved. However, the processes

in the field of near-infrared (NIR) wavelength range are still under investigation. We developed hybridized device containing quasi-2D perovskite with cadmium sulfide quantum dots (QDs) for NIR sensitive structure. It was successfully integrated with the silicon substrate. Two different patterns of the electrode materials (comb-shaped and narrow stripped) were realized by gold DC sputtering and photolithography. For the samples the spectral response, responsivity to different exposure source intensities, detectivity (normalized and angular) and response times were studied. This paper offers a promising route to optimize the performance and the electro-optical properties of the novel perovskite materials and their hybrids, and paves the path for developing high-performance electrode patterns suitable for infrared detection purposes.

1:24pm - 1:27pm

Synthesis of innovative chitosan-based functional composite adsorbents: Materials characterization and application in environmental remediation

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Restoration of the aquatic environment is nowadays a challenging task due to the presence of numerous contaminants commonly found in industrial effluents, lakes, and underground waters. Although several treatment methods have already been applied for water purification (i.e. adsorption processes), the utilization of functional composite materials as adsorbing agents is of great interest, mainly because of their structural properties that grant them exceptional adsorption abilities coupled with high mechanical strength. Notably, polysaccharides are a category of materials that have presented encouraging results in the adsorption of contaminants, with chitin along with its derivative, chitosan, being the most prominent ones. Chitosan, a biopolymer derivative of chitin, is a promising constituent for the synthesis of functional composites due to the presence of amino and hydroxyl functional groups in its structure. Materials consisting of chitosan are widely studied towards various applications including environmental restoration. Specifically, chitosan has been proven an effective adsorbent with high adsorption efficiency towards a variety of contaminants, such as heavy metals and organic contaminants. Consequently, great interest has been presented in the research for the synthesis of chitosan and chitosan-based functional composites and their application in the field of water purification via adsorption. The present study investigates the synthesis of several innovative chitosan-based adsorbents and aims to provide a comprehensive analysis of their structure and properties along with a detailed evaluation of their adsorption efficiency towards targeted water contaminants. Thus, chitosan coupled with cerium oxide or β -cyclodextrin functional composites will be produced by means of crosslinking, meticulously characterized by means of XRD, SEM, and FTIR analyses in order to assess their morphological structure and properties. Finally, the adsorption efficiency of the synthesized functional composites will be evaluated in the removal of specific contaminants, namely hexavalent chromium, indigo carmine, and brilliant black, from aqueous solutions by means of adsorption.

1:27pm - 1:30pm

The effect of prolonged exposure to elevated temperatures on the deformability and relaxation of the structure of some thermosetting polymer binders

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Present work is devoted to studying the effect of relatively prolonged exposure to elevated temperatures on the change in the deformability of some thermosetting polymer binders and glass-reinforced plastics (GRP) used for the manufacture of composite structures, such as GRP shells of chimneys and gas flue ducts of industrial enterprises. Such structures during operation are exposed to the long-term combined action of mechanical loads and elevated temperatures. The following types of binders and composites were considered: epoxy resin with an anhydride curing agent, including modified with micro-sized mineral fillers and nanosized carbon tubes; phenolic resin of the resole type; epoxy-phenolic compositions; as well as some of unidirectionally GRP. All binders and composites were cured at elevated temperatures.

As a result, the effect of holding at temperatures from 160 to 240 °C on the elastic modulus of the specimens in bending, as well as on the nature of the weight loss, was investigated. In this case, the loss of mass did not occur because of thermo-oxidative destruction; the rate of weight loss decreased when held at a constant temperature, and the sample mass is stabilized. It was found that the change in the modulus of elasticity correlates with the loss of mass of the samples. It is assumed that this is due to temperature stabilization (relaxation) of the cured binder structure, which has a domain character. The stabilization (relaxation) of the structure is presumably physical rather than chemical in nature. The following research methods were used in work: static three-point bending, dynamic mechanical analysis, thermogravimetric analysis, spectral analysis, scanning electron microscopy.

The data obtained can be used to predict the thermomechanical SSS of structures at various stages of their life cycle, as well as for artificial regulation of SSS of structures (for example, creating prestressing) by means of their heat treatment under certain conditions. The study is aimed at developing a concept that describes the relationship between the laws of formation of the thermomechanical stress-strain state (SSS) of composites with mass and energy entropy.

1:30pm - 1:33pm

Time-displaying Films Composed of Poly(N-methylaniline) and Common Transparent Polymer Films

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It is widely accepted that conductive polymer polyanilines show bright color change between their oxidized and reduced states. For example, the reduced polyaniline (PANI) looks almost colorless, while the oxidized PANI is green or purple. We have already reported

that the reduced PANI is gradually colored when it is exposed to oxygen and the coloration depends on the exposure time.¹ The color change by the oxygen exposure was brighter in poly(N-methylaniline) (PNMA) than in PANI. In this paper, several bilayer films were prepared as time-displaying films using the reduced PNMA and common transparent polymer films, low density polyethylene (LDPE), high density polyethylene (HDPE), and polypropylene (PP) films, with different oxygen permeability.

1:33pm - 1:36pm

Towards Highly Efficient Solar Cell Design Using a Dispersive Chiral Lens

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In recent work, propagation of polychromatic light through a chiral dispersive spherical boundary has been examined via deriving two sets of ABCD transfer matrices for right- and left-circular (RCP/LCP) modes [1-3]. In this work, the first-order dispersive effects via material dispersion manifested through the dielectric permittivity ϵ in a spherical lens are considered. A schematic for a chiral dispersive thick lens illuminated by white light is shown in Fig.1. Incoherent white light (sunlight) is spectrally decomposed into the constituent spectral colors. The dispersed light is then incident upon the chiral lens at location do location. The emergent multicolor waves all propagate in the meridional (YZ) plane. Consequently, based on recent work, individual colors are brought to focus by the lens to unique positions displaced in both Z and Y coordinates [4]. In the present scheme, it is proposed that individual solar cell junctions be placed to intercept each color focal points. The expectation is that in this manner, each cell will absorb a single wavelength, and hence will likely operate more efficiently. Additionally, the multi-cell configuration will undergo less thermal heating caused by polychromatic (including possibly infrared and ultraviolet) absorption.

1:36pm - 1:39pm

Two-dimensional finite quantum Hall clusters of electrons with anisotropic features

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Low-dimensional nano and two-dimensional materials are of great interest to many disciplines and may have a lot of applications in fields such as electronics, optoelectronics, and photonics. One can create quantum Hall phases by applying a strong magnetic field perpendicular to a two-dimensional electron system. One characterizes the nature of the system by looking at magneto-transport data. There have been a few quantum phases seen in past experiments on GaAs/AlGaAs heterostructures that manifest anisotropic magnetoresistance. In this work, we model the source of anisotropy as originating from an internal anisotropic interaction between electrons. We use this framework to study the behavior of finite clusters of electrons constrained in the lowest Landau level.

1:39pm - 1:42pm

Using Pulverized Waste Tire and its Activated Carbon as Adsorptive Fill Materials

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In this study, the potential of pulverized waste tires (PWTs), either on their own or derived as activated carbon, to act as adsorptive fill materials was evaluated by conducting laboratory tests for accessing their adsorption and geotechnical properties. PWT (0, 5, 10, 15, 25, and 100 wt%) was mixed with soil to evaluate the removal of BTEX components and two heavy metal ions (Pb²⁺ and Cu²⁺). Also, the efficiency of tire- derived activated carbon (TAC) using carbonization and chemical activation techniques was assessed for removal of three synthetic heavy metal ions (Pb²⁺, Cu²⁺ and Zn²⁺). The results showed as the PWT portion increased, the adsorption of BTEX was also increased. Among the mixtures, the pure PWT showed the highest adsorption capacity toward the BTEX removal with the uptake capacity for xylene, ethylbenzene, toluene and benzene were 526, 376.9, 206.6 and 126.8 $\mu\text{g}\cdot\text{g}^{-1}$ of sorbent, respectively. TAC exhibited great potential to adsorb heavy metals, with monolayer adsorption capacities as high as 322.5, 185.2, and 71.9 $\text{mg}\cdot\text{g}^{-1}$ for Pb²⁺, Cu²⁺ and Zn²⁺, respectively, which were significantly higher than the adsorption capacities exhibited by commercial activated carbon (CAC), which were 42.5, 15.0, and 14.0 $\text{mg}\cdot\text{g}^{-1}$ for Pb²⁺, Cu²⁺ and Zn²⁺, respectively. Moreover, the obtained shear strength parameters for mixing tire and soil were at a favorable range, which showed that the mixture of tire and soil could be used as adsorptive fill materials.

1:42pm - 1:45pm

Spin-Lattice Interaction in Magnetoelectric α -FeOOH

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Iron hydroxide α -FeOOH, known also as goethite, is among the most abundant iron bearing minerals in the Earth's crust. It has been known for decades as an antiferromagnetic insulator with a relatively high Neel temperature, $T_N = 120 \text{ deg C}$ [1]. Recently, on the basis of predictive DFT+U and Monte-Carlo simulations, it has been hypothesized that α -FeOOH displays significant linear magnetoelectric effect below T_N [2]. This fact revives the interest to this compound as a nonexpensive and environmentally friendly alternative to other magnetoelectric materials. So far, there is no direct experimental evidence for the suggested magnetoelectric coupling in α -FeOOH. Here we interpret the results of our recent Raman measurements on α -FeOOH, which reveal anomalous behavior of the lineshape and intensity of specific phonons near T_N [3]. On the basis of supporting lattice dynamics calculations we identify the vibrations of the bridging oxygen atoms, which mediate the spin-lattice interaction in this compound. Our results shed light on the physical mechanism of magnetoelectric coupling in α -FeOOH.



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Key Words: Magnetoelectric effect, Iron hydroxide, Goethite, Raman spectroscopy, Lattice dynamics calculations

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1:45pm - 1:48pm

Optical properties of 1D graded photonic crystals considering linear and quadratic profiles

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By using the transference matrix formalism, in this work it is presented the study of the optical properties of 1D photonic structures constructed by M periods of bilayers of dielectric material and slabs with graded index profile of two types: linear and quadratic. By varying the profile parameters, while it is preserved the average value of the refractive index for the graded slab, it is compared and describes the formation of new photonic band gaps for which its bandwidths depends on the slope and the curvature of the linear and quadratic profile respectively. Also, it is found the formation of omnidirectional photonic band gaps for the TE and TM polarization, one for the linear profile and three for the quadratic one, for which their bandwidths depends linearly on the slope and the curvature of the graded profiles. It is expected that the presented results could be useful in the construction of optical devices based in their optical response under oblique incidence.

1:48pm - 1:51pm

Laser written flexible touch-pressure sensor array based on polyimide substrate

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Flexible electronic sensors processed through straightforward laser written nanomaterials have shown promising results with unique functionality. Compared to conventional electronics that are based on rigid substrates, flexibility of the polymer materials offers thin, lightweight, low-cost, mechanical stability, and conformability. The most widely used polymer substrates for flexible electronic devices include polyethylene terephthalate (PET), polyethylene naphthalate (PEN), and polyimide (PI). Among these, PI has been a strong candidate for interfacing with flexible printed circuit board electronics due to its high thermal stability, excellent mechanical stability, and dielectric properties. Thus, flexible electronics devices with PI as a substrate material have been widely reported. A very interesting point about the PI is its ability to convert intrinsic hydrocarbons into highly cross-linked carbon structures when interacted with laser. This process is enabled either by photothermal or photophysical or even both. On the other hand, elemental carbon in different structural forms have been synthesized to fabricate various electronic devices and sensors due to their unique functional properties. Despite its unique features, straightforward synthesis, and most importantly patterning, of high quality (high conductivity) carbon structures in a scalable approach is quite challenging. To overcome this, lasers have evolved to directly write desired carbon patterns on polyimide substrates without any additional process or treatment to the substrate.

Herein, we report a flexible touch-pressure sensor with polyimide as a substrate and laser-treated carbon patterns as an interconnect and sensing elements. The laser-treated carbon film has a minimum sheet-resistance of 100 Ω/\square at a laser scanning speed of 100 mm/s, hatch spacing of 1 μm and repetition rate of 100 kHz. The sensor works based on the mutual capacitive coupling between two pair of electrodes that are of a loop and disc form. The approach also allows for the detection of proximity, touch and pressure, to enable a complete mapping of the sensor surface.

1:51pm - 1:54pm

Zn anode-based electrochromic devices

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As an emerging energy conversion technology, electrochromism has attracted immense interest due to its various applications including variable optical filters, bistable displays and energy-efficient smart windows. Although the current electrochromic devices do not consume energy while maintaining their colored or colorless states, their bistable operation requires external electrical energy to be consumed during switching. As such, a novel design of Zn anode-based electrochromic devices was recently developed as a key strategy to partially retrieve the consumed electrical energy. Compared to conventional electrochromic devices, Zn anode-based electrochromic devices show a compelling energy retrieval function. Zn-based electrochromic devices exhibit a rapid spontaneous switching behavior due to the high value of redox potential difference between a metal anode and an electrochromic cathode, thus providing the most energy-efficient consumption during operation. Moreover, Zn-based electrochromic devices enable independent operation of top and bottom electrochromic electrodes, thus providing additional configuration flexibility of the devices through the

utilization of dual electrochromic layers under the same or different color states. As such, the color overlay effect can greatly broaden the color palettes. These key issues of ZECDs make them very promising for the future development of electrochromic devices.

1:54pm - 1:57pm

Pb-substitution in Eu₃Bi₂S₄F₄: A superconductor to insulator transition

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Discovery of superconductivity in BiS₂-based compounds suggest the possibility of emergence of new high temperature superconductors from this family. They possess similar layered structure as in cuprates and iron-based pnictides. After discovery of superconductivity in Bi₄O₄S₃ (T_c = 4.5 K) various BiS₂-based systems were formed by changing the composition of block and conduction layer in the layered structure. LnO_{1-x}F_xBiS₂ (Ln = La, Ce, Pr, Nd, Sm and Yb), Ln_{1-x}M_xOBiS₂, Sr_{1-x}Ln_xFBiS₂ (Ln = La, Ce, Pr, Nd and Sm), EuFBiS₂ and Eu₃Bi₂S₄F₄ superconductors have been known. In an attempt to introduce holes in the system Sr-doping at La-sites in LaOBiS₂ was tried. But hole-doping is not found to induce superconductivity in LaOBiS₂. The structural and mixed valence properties of the Eu-based EuFBiS₂ and Eu₃Bi₂S₄F₄ superconductors have been discussed in literature. Effect of isovalent Se-substitution at S-sites leads to remarkable increase in T_c in both systems.

We have investigated effect of doping lead at bismuth site in Eu₃Bi₂S₄F₄ superconductor (T_c ~ 1.5 K). Lattice parameters and hence unit cell volume decreases gradually on increasing Pb-content in Eu₃Bi₂-xPb_xS₄F₄ (x = 0.25, 0.5, 0.75 and 1). The systematic decrease in cell volume suggests successful incorporation of Pb in the lattice. Remarkably, Pb (x = 0.25) destroys superconductivity and a highly insulating state is obtained. The susceptibility measurement shows that for x = 0.25 sample the value of magnetic moment is smaller as compared to the Pb-free compound, but in higher Pb-content the variation of magnetic moment is (±) 0.2–0.5 μB. The variation in magnetic moment in Pb-substituted samples suggest mixed valence state associated with the Eu-ions.

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1:57pm - 2:00pm

Fabrication of Uniform Green Perovskite Light-Emitting Diodes via Sandwich Evaporation Technique

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Perovskite light-emitting diodes (LEDs) have recently attracted great research attention due to their narrow emission and high color purity. The well-known methods for manufacturing perovskite LEDs are the solution process and the thermal evaporation process. Both methods are direct methods to form perovskite thin film, which may lead to an ununiform perovskite thin film due to fast crystallization. Since there are many kinds of elements to form perovskite thin film, different materials have different solubility and boiling point, each material has its own suitable parameter to form the film. Therefore, in order not to be limited by the solubility or melt boiling point of the material, we introduce a sandwich evaporation technique (SET) which combines solution method with thermal evaporation method to form the ideal perovskite thin film. In this experiment, Methylammonium Bromide (MABr) was spin-coated as the first layer of the sandwich, and then used an evaporator to deposit Lead (II) bromide (PbBr₂) as the second layer, and finally used a self-made chamber to evaporate MABr as the last layer. Finally, MAPbBr₃ perovskite thin film is then formed after annealing. In this way, it is possible to produce well crystallized, flat and uniform perovskite thin film, with narrow Full width at half maximum (FWHM) Photoluminescence (PL) spectrum under blue light stimulation. By using SET, the optimal perovskite LEDs gave the maximum luminance of ~ 392 cd/m², the maximum current efficiency of ~0.046 cd/A, and the maximum external quantum efficiency of ~0.108%.

2:00pm - 2:03pm

Optimization of the MAPb_{1-x}Cl_{3-x} Perovskite Layer in a High Performance Perovskite Solar Cell via Sandwich Evaporation Technique

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Since the implementation of perovskite material in solar cells by Miyasaka's team in 2009[1], its excellent photoelectric properties and low material cost were showcased as one of the most groundbreaking discoveries in the photovoltaic industry and other new fields of energy. With the combination of perovskite and silicon, there exists a possibility of industrializing the production of perovskite solar cells. The reason why these two materials are compatible is first due to microcrystalline silicon's energy bandgap of about 1.12 eV, which can be used in the bottom cell to absorb light from the visible spectrum to 1100 nm. In addition, perovskite has a higher energy bandgap, and when used in the top cell, can absorb the higher photon energies to generate a larger Voc. Because of minimal energy loss of photons in perovskite, the remaining photon energy will cause the excitation of electrons in silicon solar cells, maximizing the total usage of photons for solar cell efficiency. Therefore, the MAPbI₃Cl_{3-x} perovskite layer can provide an effective solution for the commercial production of perovskite solar cells. Differing from the current thin-film perovskite forming method, we developed a hand-made chamber to fabricate the perovskite layer via the sandwich evaporation technique (SET) process[2]. This process begins by first spin-coating CH₃NH₃I and thermal evaporating PbCl₂. Then, MAI is evaporated at a low pressure by the SET chamber. This device saves a lot of time in the pump-down phase and opens up the ability to form larger perovskite grains in comparison to the traditional solution method. Through the SET process, double inter-diffusion allows more complete crystals to form. The crystalline film of MAPbI₃Cl_{3-x} can be produced within 30 min.

2:03pm - 2:06pm

Add Polyvinyl Butyral to make High-Efficiency Rare-Earth-Free Fluorescent Materials

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Nowadays, the sub pixel size of displays has reached the micron level. However, Micro-LED displays cannot be easily mass-produced due to the challenge of mass transfer. In this study, polyvinyl butyral (PVB) was used with organic dyes to form a colloidal solution. By adding a specific proportion of polymer, a fluorescent film with a quantum efficiency of more than 85% can be prepared to meet the thickness of the Micro-LED for the color conversion luminescent layer (CCL). The fluorescent dyes used in our Lab are rare-earth-free fluorescent materials, so this technology will not pollute the global environment. Conventionally organic luminescent molecular films are produced by thermal evaporation deposition method. In this case, our innovative spin-coating method instead of thermal evaporation deposition method is not only conducive to large-scale production, but also beneficial for less waste of many materials. Furthermore, the use of PVB as a dispersant can make the film exhibit extremely high conversion efficiency. Moreover, the properties of PVB give the fluorescent film with good resistance to water, oxygen, acid and alkaline, so the array can not only be fabricated outside the glove box, but also resist the developer. This method results in the high brightness of Micro-LED chips and retains the high color saturation of displays.

2:06pm - 2:09pm

Study on the relationship between the degree of deacetylation and electrical and antibacterial properties of chitosan fiber and its composite yarn

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Study on the relationship between the degree of deacetylation and electrical and antibacterial properties of chitosan fiber and its composite yarn

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Functionalization of textiles by using environment-friendly materials and green manufacturing technology has been considered as a major direction of development of textile products. Chitosan fiber is a totally degradable and renewable fiber. Due to its attractive inherently antibacterial and antimicrobial properties, safety, unique characteristics for biomedical uses as well as excellent direct skin contact performance such as high level of comfort, the antiallergicity and the high humidity absorption, the applications of chitosan fiber have been extended from medical area to many other areas including textiles. However, the relationship between the degree of deacetylation and the resultant electrical and antibacterial properties is not clear, which results in the large variation of the property of chitosan fibers and the resultant fabrics, including the antibacterial and antiallergic properties. In this study, the degree of deacetylation of chitosan fiber was examined by using colloidal titration method while the electrical and antibacterial properties of fiber were evaluated following GB/T 12703.03 and AATCC 100, respectively. The fiber surface structure and cross-section, fiber length and diameter, and tensile strength and elongation were also tested according to relevant standards. Based on these results, the relationships between the degree of deacetylation and electrical and antibacterial properties of chitosan fiber can be established, and on that basis, the antibacterial mechanism of chitosan fiber can be understood. These relationships are very useful for the setup of specifications of chitosan fiber for achieving the desired antibacterial properties of the fiber and the resultant composite yarn and fabric.

Key Words: Chitosan fiber, Antibacterial property, Electrical properties, Degree of deacetylation

Acknowledgement

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2:09pm - 2:12pm

Galvanic displacement and compositional modulation in electrochemically deposited FeCoNiCuZn high entropy alloy thin films

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Galvanic displacement reactions have been revolutionary in electrochemical processes where, generally hollow, and porous metal nanostructures have been explored for several functional applications. However, this phenomenon has not been exploited for alloy systems i.e. more precisely in multicomponent alloys (MCAs) and high entropy alloys (HEAs). Of late, newer HEA systems are continuously being developed. However, HEAs containing Zn as an alloying element have not been attempted due to the complexity in mixing of low melting point elements using conventional high temperature methods. In this study, we have developed a new nanocrystalline high entropy alloy system having elements with large variation in melting points and with dissimilar crystal structures such as FeCoNiCuZn by a rapid electrochemical deposition technique in single step in aqueous medium [1]. While understanding the simultaneous deposition kinetics of five elements right after the deposition, an unusual phenomenon was observed between the electrodeposited FeCoNiCuZn high entropy alloy thin film and the electrolyte. Due to the variations in the oxidation potentials, galvanic displacement reactions have been observed between the elements in the deposited alloy and the metal ions in the electrolyte which causes compositional changes in the deposited alloy progressively at open circuit potential. This progressive change in composition occurs in the electrodeposited alloy where, copper (from ~ 10 to 55 at. %) was deposited on the alloy due to its lower oxidation potential causing displacement of Zn>Fe>Co>Ni (order of displacement) from the deposited alloy with copper ions present in the electrolyte. Morphology and modulation in composition of the HEA thin films after galvanic displacement reactions with notable variation in the copper nucleation and its coverage on the surface have been characterized by FESEM-EDS and XRD. By controlling the galvanic displacement reactions, compositionally gradient HEA thin films can be tailored which in turn can be explored for several unattempted applications. This is the first observational reporting on galvanic displacement in HEAs composed of five elements.

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2:12pm - 2:15pm

Observing and Controlling the Crystallization Process in Reconfigurable Plasmonic Superlattices

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Ordered nanoparticle solids are very interesting materials with an overarching importance for future plasmonic, metamaterial, electronic and optical applications [1]. Properties of such materials directly result from the arrangement of nanoparticles within whole volume of the material. Therefore, it is important to fully understand a mechanism of the crystallization process and answer the question how changing of various parameters and conditions affect for crystallization process. While colloidal crystallization has been thoroughly studied, for example, with advanced in-situ electron microscopy methods [2], the noncolloidal crystallization (freezing) of nanoparticles (NPs) remains so far unexplored.

To fill this gap, in our recent work [3] we performed proof-of-principle experiments decoding a crystallization of liquid-crystalline, reconfigurable assemblies of NPs at a solid state. Structure formed by these nanoparticles can be reversibly rearranged between different phases by varying the substrate temperature. To study the crystallization process we used several techniques including unique in-situ TEM, each of them give us different information about arrangement of NPs and allow us to follow the crystallization process. These experiments were repeated for materials prepared in different conditions focusing especially on cooling rate during crystallization process and number of thermal annealing cycles.

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2:15pm - 2:18pm

Influence of Rapid Thermal Annealing Time on ZnO:F Thin Films Deposited by RF Magnetron Sputtering for Solar Cell Applications

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Transparent conducting oxides are extensively used in optoelectronic devices such as photovoltaic cells, flat panel displays, optoelectrical interfaces and circuitries. ZnO-based transparent conducting thin films have been widely investigated owing to its wide direct band gap (3.37 eV), abundant raw material, non-toxicity and easy preparation at low temperature. Furthermore, its optoelectronic properties can be modified by doping with other elements. In this work, fluorine doped zinc oxide (FZO) thin films were deposited by radio-frequency magnetron sputtering from a ZnO target mixed with ZnF₂ of 3 mol%. A post-deposition rapid thermal annealing (RTA) was carried out at 300°C at annealing times varying from 0 to 120 s in vacuum with a graphite substrate as the carrier. Impact of rapid thermal annealing (RTA) on structural, electrical, and optical properties of the films were explored. The prepared FZO thin film was then used as a transparent electrode to fabricate the amorphous silicon thin-film solar cells on glass substrates, and their properties were also measured.

XRD patterns showed an intense diffraction peak at $2\theta \sim 34.4^\circ$, which suggests a hexagonal wurtzite structure with a preferential growth direction in (002) crystal orientation. The calculated grain size achieved 24.3 nm for the sample with an RTA time of 30 s with the use of the Scherrer's formula. Hall effect measurement exhibited that the film resistivity decreased by about 36% with increasing RTA time from 0 to 30 s and attained its lowest value, $7.97 \times 10^{-4} \Omega\text{-cm}$. Then it increased for a further increase in RTA time. UV-Visible transmittance spectra of thin films displayed sharp absorption edges occurred in the UV range (340–360 nm) and the average transmittance for all specimens was 91–94% in the visible region (380–780 nm). The corresponding optical band gap determined by Tauc plot increased from 3.76 to 3.83 eV after RTA treatment for 30 s. To evaluate the transparent conducting performance the Haacke's figure of merit was calculated and it enhanced by 91% to $1.92 \times 10^{-2} \Omega^{-1}$. The prepared FZO thin film was then etched by a dilute HCl solution to acquire the textured surface for enhancing light diffusion. The transmission haze ratio of the etched FZO thin film increased from 4.34% to 27.3%, but the sheet resistance almost doubled to 13.97 ohm/square. Then, p-i-n a-Si:H solar cells on the textured FZO front transparent electrode in superstrate configuration were fabricated by plasma-enhanced chemical vapor deposition at 200°C. The conversion efficiency of the solar cell with the RTA-treated FZO transparent electrode increased by 20% compared to that without RTA-treated one. These results demonstrate that RTA treatment effectively improves the optoelectronic properties of the FZO thin films, and the developed FZO thin films are suitable for transparent electrode application.

2:18pm - 2:21pm

Improvements in the efficiency of p-type bifacial Si solar cells with Cu electrode using galvanic replacement reactions

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Abstract

A novel method for fabricating the base metal Cu in an air atmosphere was successfully developed based on thick film screen printing of Al pastes and galvanic replacement reactions. The first thick film screen printed Cu electrode with high conductivity ($<10^{-6} \Omega\text{-cm}$), which is comparable to thick film Ag electrode, was successfully made in air firing instead of reducing atmosphere firing.

In this study, we introduce high-efficiency p-type bifacial PERC solar cells with an industrial typical PERC process flow used to apply a screen-printed aluminum finger grid on the rear side of an electrode instead of a full-area aluminum layer. A novel copper (Cu) technique is used to fabricate the Cu electrodes that are substituted for Al electrodes in p-type PERT c-Si solar cells. F.F. and efficiency of the p-PERT solar cell with the novel copper electrode can be remarkably improved. The maximum efficiency of the p-type bifacial single crystalline solar cells obtained with this process was 23% for the front Cu side and 20.7% for the rear Cu side illumination under standard testing conditions (STC). The ratio between front and rear side performance was over 90% for all of the solar cells.

Key Words: Thick film screen printing, chemical replacement reaction, Al, Cu, Ag, conductivity, p-type bifacial PERC solar cell

2:21pm - 2:24pm Warning: The presentations finish prior to the end of the session!

Study of Hot-Carrier Relaxation Dynamics of Cs₄CuSb₂Cl₁₂.

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In the recent years, metal halide perovskites have emerged as one of the fastest growing photovoltaics technologies. This has achieved lab-scale device efficiency of more than 23% by improving the quality of interfaces, carrier transport layers and perovskite films. Despite this tremendous progress, the organic-inorganic lead halide perovskite solar cells suffer from long-term stability, degradation and toxicity. The perovskite film is very sensitive to ambient humidity, easy to get dissolved and degraded by moisture, and has toxicity issues due to the presence of lead. Although attempts were made to stabilize the lead-based perovskite active layer there is an impetus to develop non-toxic alternatives to lead halide perovskites, with improved stability and efficiency for solar cell applications. One of the ways to get the lead-free perovskites is by substituting four Pb²⁺ cations with a divalent and two trivalent cations, for example, Cs₄CuSb₂Cl₁₂ (CCSC). This gives rise to double perovskites, which have recently emerged as viable alternatives to lead halide perovskites. Theoretical and experimental studies have demonstrated that CCSC exhibits high photo- and thermal-stability, is tolerant to humidity and its band gap values lie in the range of 1.0-1.79 eV. These properties make CCSC a suitable absorber material in solar cells. Apart from chemical and thermal stability, its magnetic response has also been explored, which shows long range magnetic ordering with anti-ferromagnetic behavior. However, the band-gap nature and excited state dynamics of these microcrystals are yet to be explored.

Here, we have theoretically investigated the electronic band structure, total density of states, dielectric constants and synthesized the microcrystals of CCSC. We have studied the different vibrational modes with Raman activity of this material. Using ultrafast transient



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absorption spectroscopy, we have explored the relaxation rates and pathways of hot-carriers. An analysis of the hot carrier relaxation process in CCSC will give us valuable information on its intrinsic carrier dynamics and further applications in solar cells.

Key words: Excited state dynamics, hot-carrier relaxation.

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FCM-5: Functional Composite Materials

Time: Friday, 20/Aug/2021: 1:00pm - 3:30pm · Virtual location: AU 2410

Session Chair: Mohsin Ali Badshah

1:00pm - 1:10pm

Properties of Carbon Nanotube Buckypaper and Interphase

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Thin-film infiltrated Buckypaper (BP) is a membrane of high CNT content nano-composites, consisting of entangled CNT networks with a porous mesh structure infiltrated with a polymeric material. The interaction between the CNT network and the surrounding polymer and between BP and the surrounding polymer in a 3-phase nano-composite occurs via interphase. This study aims to investigate the heterogeneity of BP at the nano-scale and the homogeneity at the microscale. The author uses the Atomic Force Microscopy-based Peak Force Quantitative Nanomechanics Mapping (PFQNM) technique to study the CNT BP and the CNT network interphase at the nano-scale with high lateral resolution. The trace and retrace curves of force vs. deformation response will be analyzed using Derjaguin-Muller-Toporov and Johnson-Kendall-Roberts models. Biaxial carbon fiber, Bisphenol-A/F type epoxy with amine hardener, and nonfunctionalized multiwall carbon nanotube (MWCNT) with an average outer diameter of 10-30nm, an average length of 15-30 μ m were used to fabricate BP nano-composites. The histogram of reduced modulus, adhesion, and deformation will be examined to understand the heterogeneity of BP, and the homogenized values will be compared with the static test of BP films. The size of CNT networks will be studied via. AFM and SEM. The stochastic nature of the CNT network interphase with the surrounding polymer will be investigated.

Key Words: CNT network, Buckypaper, Interphase, AFM PFQNM

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1:10pm - 1:20pm

Preparation of bismuth series visible light catalyst and its mechanism for removing Cr(VI) and organophosphorus flame retardants

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Organophosphate flame retardants (OPFRs) are characterized by stable structure and good flame retardancy, and gradually replace bromine and chlorine flame retardants in electronic products. In our research, OPFRs and Cr(VI) combined pollution as the research object to prepare high efficiency and low toxicity type visible photocatalysts. The environmental factors influencing the degradation and Cr(VI) reduction of organophosphorus flame retardants under photocatalysis were investigated. The degradation pathway and Cr(VI) reduction mechanism of organic pollutants in the combined pollution system were clarified. Explore the collaborative removal mechanism of pollutants in the combined pollution system with illumination. It provides theoretical basis and technical support for the treatment of compound pollution of organic matter and heavy metal in water environment.

1:20pm - 1:30pm

PLA- and PHBV-based Bio-composites: Improvement of the Mechanical Properties by Fiber Surface Treatment with Natural Waxes

Maria Cristina Righetti¹, Patrizia Cinelli^{1,2}, Maurizia Seggiani², Vito Gigante², Laura Aliotta², Andrea Lazzeri^{1,2}

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Thermal, mechanical and viscoelastic properties of bio-composites of poly(lactic acid) (PLA) and poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) with natural fibers (bran and potato pulp powder), untreated and treated with natural waxes (carnauba and bee waxes), were investigated.

The aim of the study was to verify a potential valorization of agri-food by-products and, in addition, to reduce the final cost of PLA- and PHBV-based materials.

The results showed that untreated bran fibers and potato pulp powder acted as fillers, and not as reinforcement, for PLA and PHBV, due to poor fiber/matrix adhesion, because a small loss in mechanical properties (tensile strength and elongation at break) was detected.

To try to improve the mechanical response, surface treatment of the natural fibers with carnauba and bee waxes was performed. This procedure was found to improve the properties of the bio-composites, enhancing the biopolymer/fiber adhesion, as confirmed also

by predictive theoretical models. In addition, the presence of natural fibers promoted biodegradation and in particular the disintegration of the bio-composites in compost.

Thus, the addition of bran fibers and potato pulp powder, treated with natural waxes, turned out to be a method useful (i) to valorize abundant agri-food by-products, according to circular economy principles, and (ii) to reduce the final cost of PLA- and PHBV-based materials.

Key Words: Bio-composites, Natural fillers, Natural Waxes, Fiber/Matrix Adhesion

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1:30pm - 1:40pm

Structural Design and Manufacturing of Three-Dimensional Porous Superstructures with Additive and Subtractive Electrochemistry for Flexible Self-Powered Electronics, Nanoelectromechanical Devices, and Water Purification

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The recent search for advanced materials with desired properties for the next-generation flexible energy devices, electronics, and environmental remediation has been focused on the unique class of three-dimensional (3D) porous superstructures that can be made of myriad materials and their composites, including 2D materials, metals, oxides, and polymers.

Herein, we report an original and rational scheme to create 3D metallic foams with tunable multi-level porosity by using a process consisting of additive electrodeposition and subtractive electroetching. The resulted metallic foams can readily serve as catalytic templates for the growth of 3D free-standing hierarchically porous thin graphite and metal-alloy-oxide composites that offer enhanced mechanical, electric, catalytic, and electrochemical performances. The feature size and morphology of the porous structure can be readily tuned and predictably fabricated with Gaussian-regression-based machine learning. The obtained materials have integrated as the flexible energy units in self-powered strain sensors and nanomotor manipulation systems, and applied for catalysis of water oxidation and water purification.

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1:40pm - 1:50pm

Spider Silks as Model Systems for the Design of Functional Protein-based Materials and Composites

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Producing synthetic materials that exhibit the outstanding physical, mechanical and functional properties of spider silk is one of the Holy Grails of Materials Science. However, researchers still lack the knowledge to reproduce the hierarchical assembly process of spider silk proteins from the liquid spinning dope to high-performance fibers in the lab. The physical and biochemical transformation processes that take place to fabricate these protein-based materials remains a complicated problem with numerous unanswered questions. The characterization of these structural and dynamic evolutions typically lack the combined experimental data that can link the atomic, molecular and meso- length scale events responsible for protein assembly into fibers. The aim of this research is to harness recent advances in magnetic resonance, cryo-TEM and simulation to develop models for the transformation of soluble silk proteins to materials that out-perform man-made systems. Solution and solid-state NMR data is being combined with data from cryo-TEM imaging and tomography and molecular dynamics (MD) simulations to begin connecting the atomic, molecular and nanometer length scales for an improved understanding of hierarchical silk formation (1).

Spiders do not produce just one type of silk fiber but, up to six distinct fibers that are all exceptional materials that vary in their mechanical properties with some tougher than Kevlar while others exhibit extensibility and elasticity analogous to rubber. Our lab is developing an understanding of the silk protein structure-function relationship that make these silks unparalleled in performance yet, highly diverse. The majority of spider silk studies have focused on the dragline silk because of its strength and toughness and ease in which it can be collected. However, prey wrapping spider silk is actually tougher than the highly touted dragline silk because of a

unique α -helical coiled β -sheet hybrid nanofiber structure (2) and exhibits a novel hydration-induced β -sheet fiber cross-linking property that we believe will provide inspiration for a new type of functional biomaterial (3).

Developing an improved fundamental understanding of the supramolecular physiochemical assembly process that enables the production of these natural materials and the global structure-function relationship across the various silks will impact applications in the defense, medical, industrial and space exploration sectors.

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1:50pm - 2:00pm

Small-Nanostructure-Size-Limited Phonon Transport within composite films made of single-wall carbon nanotubes and reduced graphene oxide sheets

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Nanocarbon materials have been widely used for nanoelectronics and other energy-related applications. In the kinetic relationship, the phonon (lattice) thermal conductivity is given as $k_L \sim C_p v_g \Lambda$, with C_p as the phonon specific heat, v_g as phonon group velocity, Λ as phonon mean free paths (MFPs). Within general composite films made of reduced graphene oxides (rGOs) and carbon nanotubes (CNTs), the existence of many nanocontacts results in a k reduction but the loss in k can be overshadowed by the significant advantages of using bulk composites for large-scale applications. Detailed thermal analysis of composite films made of rGO and CNTs is still lacking, particularly for the individual in-plane thermal conductivity ($k_{||}$) contributed from each constituent material within the complicated 3D nanocarbons. In this work, composite films consisting of rGO nanosheets and varied weight percentage of single-wall CNTs (SWCNTs) are synthesized and studied for their in-plane thermal conductivities, in which increased SWCNTs percentage leads to a reduced $k_{||}$. Different from pristine graphene and other composite nanocarbon films with decreased thermal conductivities above 300 K, the in-plane thermal conductivities of our composite films are found to follow the trend of the specific heat of graphene from 100 K to 400 K, i.e., monotonously increasing at elevated temperatures. For investigated samples, the extracted $k_{||}$ can be matched by a scaled curve for the product $C_p v_g$ summed up for all phonon modes that are computed for pristine graphene. This indicates that the rGO nanosheets contribute significantly to the $k_{||}$ but their MFPs are largely restricted by the dense SWCNT-graphene junctions and additional graphene-graphene nanocontacts. Such a trend has seldom been observed for nanocarbon. This unique temperature dependence of thermal conductivities is attributed to the so-called small-nanostructure-size (SNS) limit, at which the phonon MFPs are simply restricted as the structure size. This SNS limit is often found at cryogenic temperatures where the majority bulk phonon MFPs are much longer than the sample size. The typical size of graphene sheets divided by SWCNTs is 70–120 nm for Sample #2, and 15–30 nm for Sample #6. These sizes are smaller than the majority phonon MFPs (>100 nm) in graphene so that the phonon transport within graphene sheets approaches the SNS limit. This results in $k \approx k_L$ following the SNS limit even up to 400 K. The highest in-plane thermal conductivity among samples with different synthesis conditions is 62.8 W/m·K at 300 K, which is significantly higher than amorphous materials with a similar temperature dependence of thermal conductivities. Such a high thermal conductivity, combined with its unique temperature dependency, can be ideal for applications such as flexible film-like thermal diodes based on the junction between two materials with a large contrast for their temperature dependence of the thermal conductivity.

2:00pm - 2:10pm

Simulation of Fracture in Graphene-Polymer Nanocomposites using Molecular Dynamics

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There is now significant experimental evidence that the dispersion of a few weight percent of nanoscale particles in a polymer matrix helps to mitigate its brittleness and microcracking without incurring serious weight penalty, thereby enhancing its fracture toughness. In addition, there is further experimental evidence that particle size plays an important role in toughness enhancement. Fracture at the nanoscale is very different from the macroscale due to nonlocal effects and non-bonded interactions. Consequently, in this paper, molecular dynamics (MD) is employed to simulate the fracture process in a polymer in the presence of dispersed nanographene platelets. In the MD study presented in this paper, a 14 nm long graphene nanoparticle (GNP) is embedded in a block of thermosetting polymer EPON 862 and curing agent DETDA, having dimensions of 30.5 nm \times 31 nm \times 3.4 nm, with an edged crack of length 13.5 nm as shown in Fig. 1. This model was developed to determine the improvement of fracture properties using the atomistic J integral as a suitable metric for evaluation of toughness at the nanoscale. After densification of the system at 300K using the NPT ensemble with a pressure of 0.1 atm, the system temperature was increased in a stepwise manner from 300K to 500K using Noose-Hoover thermostat for 10 ps to enable crosslinking of the epoxy utilizing the ReaxFF force field. This resulted in a model with 80% crosslinking density and a bulk density of ~ 1.2 g/cm³. The GNP was then annealed intrinsically within the polymer block to 300K. The annealing of the polymer with embedded GNP results in slight wrinkling of the GNP, as shown in Fig 1, analogous to what is observed in experiments. The system was then subjected to uniaxial isothermal straining in the y-direction to determine its fracture properties. Also, three concentric contours around the crack was utilized to investigate the path independence of the computed J-integral. Additional MD simulations are planned where two 7 nm long GNP platelets are embedded in the polymer block replacing the single 14 nm platelet, in order to study the effect of platelet length on toughness while keeping the GNP weight percentage constant. Results pertaining to fracture toughness properties for both cases will be presented.

2:10pm - 2:20pm

Cell Membrane-Covered Hybrid Nanocomposites for Target Photothermal Cancer Therapy

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The so-called theragnostic materials represent the state-of-the-art in the use of nanocomposites for targeting cancer diagnosis and treatment. Graphene oxides and gold nanorods (AuNRs), in particular, have been extensively applied as theragnostic agents for target cancer therapy due to their ability to absorb light in the near infrared region - where radiation penetration through tissues occurs-, which makes them appropriate for in vivo photothermal applications. In this paper we show the development of AuNRs covered with lung adenocarcinoma cell (A549) membranes, used for targeting and photohyperthermia essays in vitro and in vivo. The nanoconjugates presented higher toxicity to cancer cells compared to healthy cells used as controls. Additionally, significant differences were observed on how the AuNRs interact with the cancer and normal cells, as revealed by kinetics absorption and surface pressure measurements in Langmuir experiments. Our results show the potential of cell membrane-coated nanomaterials and open opportunities for the development of more efficient nanosystems for cancer applications.

2:20pm - 2:30pm

Development of Novel Self-Centering Polyurethane Piston Based Bracing

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In braced frames, the response of a structure after an earthquake can be affected by the bracing system's strength and properties. Concentric Braced Frames (CBFs) are mostly used to resist the seismic load. However, traditional tension-compression bracing system may not perform well under earthquake loads because of buckling in compression. Other bracing systems such as Buckling Restrained Bracing (BRBs) and are being used to solve this problem. Buckling restrained braces are one of the practical systems to resist seismic loads. However, they cannot prevent permanent deformation in the building. To overcome the shortcomings of the developed system, a new Polyurethane Piston Based Bracing (PPBB) system has been developed and fabricated at the University of British Columbia. This device consists of a brace system that can take a considerable tension and compression force. The system is a cylinder-piston assembly in which polyurethane and steel are utilized. This specimen consists of five main parts: two halves of steel tubes, two polyurethane cylinders and a shaft. Quasi-static as well as strain rate experimental testing was performed on the device where very good self-centering behaviour was achieved using this relatively cheap and light material. This was achieved by analyzing the Displacement versus Force graph and finding the energy dissipation for this system.

2:30pm - 2:40pm

Evaluation of impurities concentration with hot probe method and optical constants of nanostructured titanium dioxide embedded polymer thin films

Nafeesah Abdulrahim Yaqub, Aslam Farooq Wazirzada, Mohammad Al Salihi

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Electrical and optical characteristics of nano particle embedded polymer thin films significantly differ from those of pure polymers. Therefore, characterization methods for evaluation of nano particle embedded polymer thin film became highly important. A novel approach to the well-known "Hot-Probe" method is applied in present work. The conventional Hot Probe characterization method enables the definition of a semiconductor type, P or N, by identifying the majority charged carriers. According to the Hot Probe technique, one can measure and calculate the majority charged carriers concentration and its dynamic parameters. In the present report evaluation of majority charged carriers concentration of nano sized titanium dioxide embedded PMMA polymer is carried out with Hot Probe technique. The polymer samples are prepared with various concentration of nano sized titanium oxide using casting method. Optical constants of these samples are also determined using transmission and reflection curves in wide range of wavelengths.

2:40pm - 2:55pm

Ferroelectric Nanocrack-based Nanoelectromechanical Switches for Memory and Complementary Logic

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The power consumption is one of the most challenging bottlenecks for electronic devices. Nanoelectromechanical (NEM) switches offer a promising platform to break the Boltzmann Tyranny and thus enable to construct energy-efficient electronic devices. NEM switch enables near-zero leakage current and steep subthreshold slope relying on the electrostatic force to form or remove an air gap between source and drain, but usually has a much complex structure [1,2]. Therefore, We constructed a NEM switch with a controllable ferroelectric-nanocrack employed (001)-Pb(Mg1/3Nb2/3)0.7Ti0.3O3 (PMN-PT) substrate/Mn50Pt50 heterostructure, which offers a simple and efficient way to manipulate the device resistance states with a high on/off ratio [3]. Meantime, ferroelectric devices utilize the polarization switching through voltage-control, offering great advantages in non-volatility, scalability and energy-efficiency. Such devices we proposed combine the advantages of nanoelectromechanical (NEM) switch and ferroelectricity. Further, the complementary switching of nanocracks has also been revealed and investigated, which operates like the CMOS technology [4,5]. Based on the ferroelectric-nanocrack NEM switch, we condense the memory and logic functions into a single device. Superior electrical performances in both on and off states have been demonstrated with metallic contacts at on state and zero off-state leakage current. Importantly, we focus on the scaling performance that is crucial for actual applications and find that the operating voltage can be largely reduced to average 2.5 V with device scaling down to sub-micrometers (300 nm node). Moreover, we predict sub-1 volt can be acquired at 100 nm nodes. In addition, a variety of logic gates including NOT, 2:1 MUX, AND and OR functions have been

experimentally demonstrated in a single device, leading to less chip area consumption compared to the conventional CMOS technology.

2:55pm - 3:05pm Warning: The presentations finish prior to the end of the session!

STUDY OF EFFICIENCY OF IONIZING RADIATION IN PBAT/PLA BLEND REINFORCED WITH BIO-EGGSHELL

Elizabeth Carvalho Leite Cardoso, Duclerc Fernandes Parra, Sandra Regina Scagliusi, Ademar Benevolo Lugão

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Plastics global annual production exceeds 300 million tons and 99 % of the total plastic production is originated from oil or other fossil combustibles. When discarded, plastics oil based can last by centuries, posing a great threat for society and when burned, they release carbon dioxide in atmosphere, contributing for a global climate change. As an alternative, they are being slowly replaced by bioplastics, as PLA (poly-lactic acid) and PBAT (butylene adipate co-terephthalate). Food and dairy industries produce annually huge amounts of avian eggshells residues and their disposition constitute a serious environmental risk. Bio-load from avian eggshells as polymers reinforcement are based in their higher benefits as resistance and rigidity besides being a friendly environmental material, degradable and renewable. PLA and PBAT are thermoplastics capable to be processed by conventional methods: nevertheless, due to their high interfacial tension, it is required the use of compatibilizers. In this work, additives and heat generally used as compatibilizers were replaced by ionizing radiation: electron beam and gamma radiation, at 200 kGy dose. It was used PBAT/PLA 50/50, with avian bio-eggshell (bio-CaCO₃), 125 µm particle size, along with compatibilizers. Characterizations included: DSC, TGA, FTIR, XRD and mechanical essays.

Keywords: avian eggshell, PBAT, PLA, electron-beam, gamma-radiation.

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EPMM-INV-4: Electronic, Photonic and Magnetic Materials

Time: Friday, 20/Aug/2021: 1:00pm - 4:00pm · Virtual location: AU 2412

Session Chair: Orion Ciftja

1:00pm - 1:15pm

Embedded metal nanoparticles: shape engineering, electronic and magnetic properties, an experimental and theoretical investigation

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Metal nanoparticles (NPs) embedded in a thin dielectric medium is a class of materials those have shown promising applications in various scientific and technological fields. Ferromagnetic metal-insulator (FM-I) granular films have attracted a considerable attention because they exhibit a wide variety of interesting properties in magnetism and magneto-transport, which suggest their attractive applications like information storage, shielding and bit writing at high frequencies, MR sensors and read heads, high sensitivity Hall sensors, field emission and solar energy applications.

In the present work, Ni: SiO₂ (Ni nanoparticles embedded in SiO₂ matrix) and FeCo: SiO₂ (FeCo nanoparticles embedded in SiO₂ matrix) granular films of various metal atomic fraction (x) have been prepared by Fast atom beam (FAB) sputtering technique and their structural, electrical, magnetic, magneto transport and field emission properties have been studied.

The following results have been highlighted in the talk: (i) Enhanced extra ordinary Hall effect (EHE) in Ni-SiO₂ films, (ii) Tunneling magnetoresistance in FeCo-SiO₂ films, (iii) exchange bias effect in FeCo-SiO₂ films and (iv) enhanced field emission current density from shape engineered FeCo NPs embedded in SiO₂ matrix. An in-depth analysis of the results have been carried out using state of the art experimental techniques and density functional theory (DFT) based calculation. Finally, prototypes developed using these materials will be shown.

Keywords: Metal-insulator nanocomposites, Extra ordinary Hall effect, Tunneling magneto resistance, Field emission, Exchange bias, Density functional theory

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1:15pm - 1:30pm

Nanomagnetism and spintronics of Cr₂O₃ thin-film magnetoelectric antiferromagnets

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Thin film magnetoelectric antiferromagnets (AF) is a viable material science platform for prospective high speed and energy efficient spintronic devices for memory and logic applications. To explore their application potential, it is necessary to understand modifications of the magnetic properties of AF thin films with respect to their bulk counterparts. Here, we will discuss spintronics, magnetometry and microscopy of bulk α -Cr₂O₃ single crystals [1] and relate them to the properties of α -Cr₂O₃ thin films [2-5]. In transport experiments, we access the magnetic state of the Cr₂O₃ relying on the spin Hall physics in a Pt thin film brought in proximity to the insulating antiferromagnet [2-4]. The analysis of the transport data is backed up by the real space imaging of AF domain patterns using NV microscopy [1,5]. Considering grainy morphology of thin films, we address questions regarding the change of the intergranular exchange [5], criticality behavior and switching of the order parameter [2] and physics of the readout signal in α -Cr₂O₃ interfaced with Pt [3]. In particular, the possibility to read-out the antiferromagnetic order parameter all-electrically enables a new recording concept of antiferromagnetic magnetoelectric random access memory (AF-MERAM) [3]. Furthermore, relying on the elasticity of antiferromagnetic domain walls in Cr₂O₃ single crystals and exploring their efficient pinning at lithographically defined mesa structures, the concept of domain wall based antiferromagnetic memory was put forth [1].

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1:30pm - 1:45pm

Cellulose-based composite materials for additive manufacturing in electrical insulation, automotive and marine industries

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As the awareness on resource sufficiency, climate change mitigation and circularity of materials increases globally, many industrial sectors are currently looking for novel solutions in replacing fossil-based materials. Cellulose as a nature-based, sustainable and versatile material is a potential replacement for many synthetic materials. In addition, cellulose has many unique inherent properties that make it interesting for novel type of applications, beyond the obvious ones, such as paper and board. However, when considering the combination of cellulose and additive manufacturing (AM), one challenge is painfully obvious: cellulose is not thermoplastic by nature.

This challenge is currently being addressed in an EU funded project NOVUM, eventually targeting at building a pilot line suitable for producing components from cellulose-based composite materials by AM for versatile applications. During the project lifetime, the process will be demonstrated for electrical insulation, marine and automotive industries. For electrical insulation components, cellulose is a common raw material but the state-of-the-art production method is rather inefficient in terms of labor, time, energy and waste generation. Additive manufacturing presents an appealing technology for boosting the process. For marine industry, the use case would be something completely new - on-demand printing of outdoor decorative elements for cruise ships. For automotive industry, the key motivation is the increase in sustainability, which the replacement of fossil-based materials with bio-based ones will bring about.

The thermoplastic cellulose-based composite materials developed in the project contain cellulose derivatives, such as cellulose acetate propionate, microcellulose and bio-based plasticizers. They have a higher cellulose content (up to 60%) than the commercial references but the material strength properties are at the same level or even better. The material properties can be tuned according to the requirements of the end use. The materials have excellent printability using commonly available printing technologies such as Fused Deposition Modelling (FDM) and light and have a smooth surface. The composite materials can be printed as granules and there is a possibility for recycling and reuse of the material by crushing and granulating, without the need of compounding prior to printing, thus contributing to the circularity of the materials.

1:45pm - 2:00pm

PEEK- A high-performance polymer used as patient-specific implants

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PEEK (polyetheretherketone) which is a high-performance polymer has great potential as using patient-specific implants in the field of medicine and dentistry because of its biocompatible properties. Recently, patient-specific implants are common due to their best fitting components with the anatomical structures. In addition, patient-specific implants fabricated from PEEK are common in the field of plastic surgery applications. On the other hand, the intraoral applications of PEEK are rare and limited to intraoral implant-supported prostheses. PEEK implants or frameworks are fabricated by subtractive technologies. However, patient-specific implants should fit the anatomy. Therefore, patient-specific implants require complex design which should be fabricated by additive manufacturing known as 3D printing.

In this report, the possible applications of patient-specific implants fabricated from 3D-printed PEEK will be discussed with rare case reports and treatment outcomes as well as finite-element analysis reports. Material properties as well as future applications of PEEK –a high-performance polymer- will be introduced.

2:00pm - 2:15pm

Ferroelectric Phase Transitions in Strained K_{0.9}Na_{0.1}NbO₃ Epitaxial Films Studied by in situ X-Ray Diffraction and Three-Dimensional Phase-Field Simulations

Martin Schmidbauer¹, Laura Bogula¹, Bo Wang², Michael Hanke³, Leonard von Helden¹, Adriana Ladera^{2,4}, Jian-Jun Wang², Long-Qing Chen², Jutta Schwarzkopf¹

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A high-temperature phase transition in strained ferroelectric K_{0.9}Na_{0.1}NbO₃ thin films epitaxially grown on orthorhombic (110) NdScO₃ substrates is identified and investigated both experimentally by three-dimensional in situ X-ray diffraction and theoretically by three-dimensional phase-field simulations. At room temperature, the thin films show a strongly anisotropic misfit strain that induces the appearance of monoclinic a1a2/MC phases. This phase coexistence leads to the formation of a regular, herringbone domain pattern. With increasing temperature, a ferroelectric-to-ferroelectric phase transition to an orthorhombic a1/a2 phase takes place. This is accompanied by a regular stripe domain pattern with exclusively lateral electric polarization. Corresponding simulations of the scattered X-ray intensity patterns show that the orthorhombic unit cells exhibit a small in-plane rotation. This leads to four different in-plane orientations of the orthorhombic unit cells and, correspondingly, to four variants of superdomains. The experimental results are fully consistent with three-dimensional phase-field simulations using anisotropic misfit strains. This applies in particular to (i) the three-dimensional domain wall arrangement in room and high-temperature phases and (ii) the broad phase transition range between about 180 °C and 260 °C, where a complex interplay of coexisting monoclinic a1a2/MC and orthorhombic a1/a2 phases occurs [1,2].

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2:15pm - 2:30pm

Using graphene-based devices and interconnects for IC Reliability

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This is an Invited talk

2:30pm - 2:45pm

Damage assessment of composites using techniques based on guided waves and electromechanical impedance

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In the presented research the guided waves (GW) propagation as well as the electromechanical impedance (EMI) were studied in the context of non-destructive evaluation (NDE) and structural health monitoring (SHM) of structural parts made of composites. Both techniques are employing piezoelectric transducers for actuation the structure and sensing the response. The focus in this research was put on relatively thin walled structural parts made of carbon fiber reinforced polymers (CFRP) as well as glass fiber reinforced polymers (GFRP). Multi-modal nature, dispersion, and direction dependence of guided waves propagation was considered for developing the damage detection tools. The results present the behavior of the waves influenced by the reinforcing fibers orientation, presence of the stiffener, as well as the presence of the damage. Moreover, in order to study the wave propagation phenomenon in detail, the scanning laser Doppler vibrometer (SLDV) was employed allowing to visualize the whole wave field of the propagating waves. In the area of electromechanical impedance the range of sensitivity was studied and the effective frequency range needed for the damage assessment. Both techniques analyzed in this work depend greatly on the sensor placement on the inspected object. This topic was addressed by considering representative examples of sensor networks and performing damage localization using them. The signal processing procedures developed for damage assessment were analyzed and the advantages and disadvantages of the procedures were highlighted.

2:45pm - 3:00pm

Halide perovskites for applications in nanophotonics

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Nanophotonics and meta-optics based on optically resonant all-dielectric structures is a rapidly developing research area driven by its potential applications for low-loss efficient metadevices. Recently, the study of halide perovskites has attracted enormous attention due to their exceptional optical and electrical properties. As a result, this family of materials can provide a prospective platform for modern nanophotonics [1] and meta-optics [2], allowing us to overcome many obstacles associated with the use of conventional semiconductor materials. Here, we overview the recent progress in the field of halide perovskite nanophotonics starting from single-particle light-emitting nanoantennas [3,4] and nanolasers [5] to the large-scale designs working for surface coloration, anti-reflection, and optical information encoding [6-8].

3:00pm - 3:15pm

Colloidal Photonic Crystals: Mind the Gap!

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Colloidal particles in the size range of hundreds of nanometers appeal as building blocks for photonic crystals with a complete photonic band gap in the visible [1]. The self-assembly of colloidal photonic crystals, despite being promising as a low-cost, scalable fabrication route, has proved elusive over nearly three decades of research [2,3]. The most sought-after colloidal photonic crystals are rather open, comprising low-coordinated colloidal particles, making them challenging targets for programmed self-assembly [4]. Additionally, stacking faults in these self-assembled colloidal open crystals tend to compromise their photonic band gaps [2,3]. In this presentation, I will demonstrate, using a variety of computer simulation techniques, how hierarchical self-assembly pathways for triblock spherical patchy particles via the so-called colloidal molecules can be exploited to address these long-standing issues [5-7]. Moreover, I will establish that triblock patchy rods can be exploited as designer building blocks for a certain colloidal open crystal to support a photonic band gap robust to stacking faults, while hewing closely to current experimental constraints [7]. I will discuss how our design rules alleviate issues that have impeded the success of colloidal self-assembly as a bottom-up means of fabrication of photonic crystals for visible light management [6,7].

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3:15pm - 3:30pm

Ionic Liquids Based Colloidal Solutions as Nanoreactors for Advanced Materials

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Room temperature ionic liquids (RTILs) are the organic analogues of inorganic molten salts with melting temperature <100°C [1]. Being ionic in nature, these compounds are versatile in terms of solvent properties such as low volatility, high thermal stability, wide liquid range and good solvating ability. In view of flexibility of choice of cations or anions, RTILs can be designed as low viscosity media suitable for self-assembly of amphiphile molecules or also can be designed as surfactants by incorporating amphiphilic character in either cation or anion or in both the constituents. Therefore, with extraordinary properties it has been possible to include RTILs as media or as surfactant or both for preparation of colloidal formulations/self-assembled structures [2]. Such structures are highly thermally stable and can be used as recyclable templates for preparation of shape/size controlled nanomaterials/quantum dots/metal organic frame works (MOFs), carbon dots (CDs) and hybrid materials [3,4]. We have constructed a stable ionic liquid colloidal system, where low viscosity ethyl ammonium formate IL is used as medium, R (+) limonene as non-polar medium, and bio-based surface active Choline[AOT] as an amphiphile. Self-assembled structures, thus constructed, have been utilized as recyclable nanoreactors for synthesis of a variety of shape and size controlled MOFs viz. HKUST-1, UiO-66-NH₂, ZIF-8, and MIL-53(Al)-NH₂ at room temperature in a generalized approach. The synthesized MOFs have been studied for gas adsorption and preparation of composite membranes for mixed salt separation applications.

Key Words: Ionic Liquids, Colloidal Systems, Nanoreactors, Advanced Materials

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3:30pm - 3:45pm Warning: The presentations finish prior to the end of the session!

Vortex nanostructures: from micromagnetic simulations to cancer cells internalization for magneto-mechanically induced damage applications.

Celia Tavares de Sousa¹, Ricardo Magalhaes¹, Sofia Caspani¹, Suellen Moraes¹, Ludgero Peixoto¹, David Navas², Carolina Redondo³, Rafael Morales^{4,5}, Sofia Lima⁶, Claudia Nunes⁶, Salette Reis⁶, Joao Pedro Araujo¹

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Novel magnetic nanostructures (MNS) present a unique spin arrangement in the magnetic ground state, namely spin-vortex or synthetic antiferromagnetic state. They are not spherical, rather disc or wire-shaped. MNS showed promising results in cell separation, as a contrast enhancing agents in MRI and in magneto-mechanically induced cell annihilation. The main advantages of magneto-mechanically induced cell annihilation are the usage of weaker magnetic fields with lower frequencies, as well as the need for a lower concentration of particles [1].

In this work, we developed one subset of biocompatible magnetic nanostructures that exhibit a spin-vortex state with interest in analysing their application in magneto-mechanically induced cell death. First, micromagnetic simulations, using mumax3 of sub-micron iron discs, were performed for different interdot distance and aspect-ratio (thickness/diameter). By analysing the nucleation and annihilation fields, as well as the magnetic susceptibility, it was found that the (ideal) discs could be considered as isolated for interdot distances greater than twice the radius of the disc (2R) [2]. We also found that discs with an aspect ratio between 5 and 15 should sustain the vortex state in remanence.

Iron nano-discs, with a diameter of about 500 nm, were fabricated by electron beam evaporation on a Si substrate pre-patterned by interference lithography [3]. The discs, protected by bottom and top gold layers, were fully characterized and the obtained magnetic measurements are in good agreement with the micromagnetic simulations. Then, the magnetic vortex nano-discs were released from the substrate by chemical etching of a sacrificial layer. Subsequently, cell viability and uptake assays were performed in a human leukaemia monocyte cell line (THP-1). Several concentrations of nano-discs were studied by flow cytometry. As a result, the discs were internalized by the cells and found to be innocuous to them, in the absence of an external magnetic field.

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