

Meeting Abstracts

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Keynotes

Welcome the Spring of the Third Milestone in Pharmaceutical Drug Development: RNA Therapeutics

Peixuan Guo

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Abstract:

RNA nanotechnology is the bottom-up self-assembly of nanometer-scale architectures, resembling LEGOs, composed mainly of RNA. The ideal building material should be (1) versatile and controllable in shape and stoichiometry, (2) spontaneously self-assemble, and (3) thermodynamically, chemically, and enzymatically stable with a long shelf life. RNA building blocks exhibit each of the above. RNA is a polynucleic acid, making it a polymer, and its negative charge prevents nonspecific binding to negatively charged cell membranes. The thermostability makes it suitable for logic gates, resistive memory, sensor set-ups, and NEM devices. RNA can be designed and manipulated with a level of simplicity of DNA while displaying versatile structure and enzyme activity of proteins. RNA can fold into single-stranded loops or bulges to serve as mounting dovetails for intermolecular or domain interactions without external linking dowels. RNA nanoparticles display rubber- and amoeba-like properties and are stretchable and shrinkable through multiple repeats, leading to enhanced tumor targeting and fast renal excretion to reduce toxicities. It was predicted in 2014 that RNA would be the third milestone in pharmaceutical drug development. The recent approval of several RNA drugs and COVID-19 mRNA vaccines by the FDA suggests that this milestone is being realized. Here, we review the unique properties of RNA nanotechnology, summarize its recent advancements, describe its distinct attributes inside or outside the body, and discuss potential applications in nanotechnology, medicine, and material science.

Mechanisms of Reductions Catalyzed by M(0)-nanoparticles

Dan Meyerstein

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Abstract:

Borohydride is often used as a reducing agent. However, the reductions of halo-organic compounds, nitro-aromatic compounds, bromate *etc.* require a catalyst. M^0 -nanoparticles, M^0 -NPs, and M^0 -NPs entrapped in sol-gel matrices are commonly used as the catalysts, where M = Ag or Au are often used. Recently it was shown that Fe⁰-NPs entrapped in sol-gel matrices can replace the more expensive metals. It is commonly accepted that the first step in the catalytic reduction with borohydride is:

1. $BH_4^- + M^0 - NP + 4H_2O \rightarrow B(OH)_4^- + (M^0 - NP) - H_4$

The next steps depend on the substrates. In the case of halo-aliphatic substrates, RX, it is proposed that the first products are H_3O^+ , X⁻and R⁻. The radicals R⁻react with the M⁰-NPs forming intermediates of the type R-M⁰-NPs or R_n-M⁰-NPs. The mechanisms of decomposition f the latter intermediates depend on the nature of substituents on R, on the nature of M, on the concentration of BH₄⁻ *etc.*

However, recent DFT analysis points out that at least for M = Ag reaction (1) does not occur. These results raise the question whether the catalyzed reductions do not proceed via the formation of $(BH_4^-)_n$ -Ag⁰-NPs and that the adsorbed borohydride is the active reducing agent.

Chemistry Beyond Conventional Wisdom

Puru Jena

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Abstract:

The chemistry of elements in the periodic table, created by Mendeleev in 1869 before the discovery of the electron and the knowledge of quantum mechanics, can be explained in terms of their valence electrons and the orbitals they occupy. For example, noble gas atoms, with filled outer electron orbitals (ns2 np6) are chemically inert. Similarly, zinc, with an outer electron configuration of filled s shell (4s2), is divalent and interacts weakly with another Zn atom. But bulk Zn is not chemically inert; it is metallic. Noble gas atoms forming chemical bonds at room temperature and zinc assuming an oxidation state of +III are against conventional wisdom. In this talk, I will discuss ways in which zinc can be in a +III oxidation state and noble gas atoms, including argon, can form a covalent bond at room temperature. These unexpected features are made possible by the use of highly stable super-electrophilic clusters. In particular, BeB11(CN)12 and BeB23(CN)22 clusters, which are, respectively, stable as tri-anion and tetra-anion in the gas phase, can make Zn to assume +III oxidation state. On the other hand, B12(CN)11- cluster can bind argon with a binding energy of 0.6 eV. These results, based on density functional theory with dispersion correction, have predictive capability and provide a path to manipulate text book chemistry. The rational design of clusters with electron affinities far exceeding those of halogen atoms and their ability to promote chemical reactions once thought impossible can usher a new era in chemistry and materials science.

*Work supported by the Department of Energy

Featured Presentations

Orally Targeted Delivering Drugs to Diseases

Xing Zhou

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Abstract:

Targeting of nanoparticles to distant diseased sites after oral delivery remains highly challenging, due to the existence of many biological barriers in the gastrointestinal tract. Here we report targeted oral delivery of diverse nanoparticles in multiple disease models, via a 'Trojan horse' strategy based on a bioinspired strategy using solvable or unsolvable beta-1.3-glucose). Diverse nanoprobes or nanotherapies are efficiently packaged into YC or coated with beta-1.3-glucose (laminarin) through electrostatic force, resulting in different diagnostic or therapeutic assemblies. Post oral administration, nanoparticles coated with beta-1.3-glucose are first transcytosed by M cells and sequentially endocytosed by macrophages, then transported to neighboring lymphoid tissues, and finally delivered to remote diseased sites to locally exert their designed functions, all through the natural route of macrophage activation, recruitment, and deployment. Through this intricate transportation route, nanoprobes or nanotherapies can be preferentially delivered to desired sites, which affords remarkably improved efficacies for the treatment of multiple diseases associated with inflammation, such as tumor, inflammation, high-fat-diet-induced obesity, insulin resistance, fatty liver and atherosclerosis.

Engineering of Nanomaterials for Drug Delivery and Bio-Sensing

Beatrice Fortuni

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Abstract:

In the last decades, nanotechnology has made impressive advances in cancer therapy, however cancer remains one of the leading causes of death worldwide, with only a very few of the nanosystems developed reaching the clinical trials. This disappointing steady state indicates that there is an enormous gap between research and clinics. Too often results obtained by in cellulo experiments are not reproducible in in vivo studies. The research presented here aims to contribute filling in this gap by deeply investigating what happens intracellularly when drug delivery systems are introduced. The strategy is two-fold: (i) developing innovative and very efficient drug delivery systems and deeply studying their intracellular dynamics, and (ii) proposing an alternative advanced system to investigate the intracellular environment with a unique spatio-temporal resolution. A multifunctional drug delivery system, based on doxorubicin-loaded mesoporous silica nanoparticles coated with polyethylenimine and hyaluronic acid, was developed. The system exhibited cancer targeting, endosomal escape capability, intracellular controlled drug release and high therapeutic efficiency. Differently, an innovative carrier-free drug delivery systems, exclusively made of prodrug has been introduced, so called nanoprodrug. FRET properties were introduced in the nanoprodugs to study their intracellular degradation and enzymatic digestion via FRET. On the other hand, we developed an innovative technique to investigate the intern of a living cell, by using Silver Nanowire-mediated endoscopy. This technique showed great potential to uncover crucial insights into cancer cells and their response to treatments.

Chlorogenic Acid Nanoemulsion: As an Effective Skin Whiting Formulation

Yasemin Budama-Kilinc

Yildiz Technical University, Turkey

Abstract:

Tyrosinase plays a significant role in melanin biosynthesis. Tyrosinase inhibitors can also be used for treatment of hiperpigmentation due to preventing melanin accumulation in the skin. Chlorogenic acid is the one of the polyphenolic compound which is a natural tyrosinase inhibitor, and it can be use for hyperpigmentation treatment. However, due to the CA is hydrophilic, it is required to enhance intradermal delivery to apply CA effectively for topical purposes.

In this study, CA nanoemulsion formulation was developed and characterized. Its conrolled release profile was determined. In addition, the safety test was conducted in vitro cell culture with cytotoxicity test. Moreover, the efficacy of the CA-NE formulation was evaluated by using tyrosinase activity test in vitro cell culture, and molecular docking studies in silico methods.

In the light of all our results obtained with in vitro and in silico studies, it was thought that the CA-NE formulation might hold promise for cosmetic applications such as skin lightening.

Nanocomposites of Nylon 6 and Carbon Nanoparticles Modified with Aminos and Acids Groups for the Adsorption of Uric Acid

Christian Javier Cabello Alvarado

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Abstract:

There are currently 850 million patients; the hemodialysis process is carried out by means of an extracorporeal circulation that allows to eliminate toxins and liquids from the blood through the membrane that constitutes the dialyzer. The following work presents the obtaining of a polymeric nanocomposite based on nylon 6 with graphene nanoplates and carbon black modified with amino and acid groups, as an adsorbent for uremic toxins. The modification of the nanoparticles was carried out by means of variable frequency ultrasound with frequency ranges of 15-50 kHz, and the obtaining of the compounds was realize by ultrasound-assisted extrusion. The polymeric nanocomposites were characterized by FTIR, TGA, DSC, SEM microscopy and adsorption isotherms, to see the removal of uric

acid. In the results of the FTIR characterizations, the signal of the NH group, belonging to the amino and acid groups, and the signals of the nylon 6 polymer can be seen. In TGA and DSC, a small increase in thermal stability could be observed. by adding the modified graphene and carbon black nanoparticles. Through SEM microscopy, an adequate dispersion of the carbon particles in the nylon 6 polymer matrix can be observed. The materials were tested as adsorbent material for uremic toxins using UV-Vis spectroscopy and hemodialysis conditions, obtaining a removal percentage of 80.35% of uric acid.

Preparation and Application of Multifunctional Nanoparticles with Hemostasis and Regulating Blood Coagulation

Qing Zhang

Chongqing University of Technology, China

Abstract:

Trauma and coagulation dysfunction can cause uncontrollable massive bleeding, resulting in death. Therefore, hemostasis has important clinical significance in prevention, operation and emergency. However, while controlling bleeding, thrombosis caused by platelet activation and aggregation can not be ignored. Thrombus affects the blood circulation of the body and leads to cardiovascular diseases. Therefore, there is an urgent need for an advanced hemostatic material with the dual functions of rapid hemostasis and regulating blood coagulation. The positively charged Polylysine and non-steroidal anti-inflammatory drug Sulindac were self-assembled to form nanoparticles. When there is bleeding in the body, the nanoparticles can activate platelet aggregation and promote the formation of clots by releasing Polylysine. Sulfides metabolized by Sulindac in the body inhibit the high aggregation of platelets, thus sequentially regulate the blood coagulation state, promote the blood coagulation function in the early stage of hemostasis, and exert the hemostatic function. After the end of hemostasis, inhibit blood coagulation, reduce the risk of hypercoagulability and thrombosis. The nanoparticles can achieve the functions of hemostasis and regulating blood coagulation.

Inorganic Nanoparticles in Drug Delivery

Tanya Singh Jamia Hamdard, India

Abstract:

Inorganic nanomaterials feature a wide variety of attributes that make them highly promising candidates for drug delivery. The inorganic component of these materials imparts unique properties to the resultant systems, providing access to new properties and capabilities for both delivery and imaging applications. Inorganic structures also provide scaffolds for the presentation and encapsulation of drugs, biomolecules, and imaging agents, generating delivery systems with structural and dynamic properties complementary to more conventional polymeric and lipidbased delivery vectors.Nanomaterials can be fabricated with a wide range of magnetic properties that likewise derive from their nanoscale dimensions. In addition to their physical properties, nanomaterials provide access to a diverse array of shapes and morphologies. For instance, the use of nanoporous silicon produced via etching of Si, including both silicon and silicate systems produced via oxidation of silicon precursors. In these systems the pores serve as carriers for drugs and polymers, while the microparticle 'mothership' can be used to target the therapeutic to disease sites.

We can therefore conclude that nanomaterials have much to offer in biomedical applications. While there are clearly hurdles to be overcome in implementing these systems as delivery vehicles, their unique attributes and ease of production will make these nanosystems important additions to our toolkit.

The Development of a Multifunctional Drug Delivery System for Efficient Cancer Cell Targeting in 3D Cell Models

Indra Van Zundert

KU Leuven, Belgium

Abstract:

Despite significant advances in cancer research, cancer remains one of the major causes of death worldwide. Commonly used treatments show serious side effects and are often ineffective, leading to the development of alternative treatment approaches in which cancer cell specificity and high efficacy prioritize. In the present study, a multifunctional targeted drug delivery system (DDS) was designed that combines specific targeting to cancer cells and endosomal escape capabilities. Mesoporous silica nanoparticles (MSNPs) were functionalized with polyethyleneimine, a polymer that is able to induce a rupture of the endo/lysosomal membrane, and conjugated to an anti-CD44 antibody, that binds to the CD44 receptor (overexpressed in many cancer cell types) inducing receptor-mediated endocytosis of the DDS. Our DDS was evaluated in 2D cell cultures, confirming their specificity and endosomal escape capability, and in more advanced 3D multicellular spheroid models. Studies in spheroids reveal equal targeting ability in this more complex 3D model when comparing CD44 overexpressing and non-CD44 expressing spheroids. In addition, satisfactory results were found regards penetration depth in spheroid models

Nanomedicine and Brain Diseases

Giovanni Tosi

University of Modena and Reggio Emilia, Italy

Abstract:

The research of non-invasive therapy for the treatment of neurodegenerative diseases is one of the most important topics of the last years by the pharmaceutical technology. Even if less than 1% of both industrial and university research projects on neuroscience displays of a Blood-Brain Barrier (BBB) crossing and CNS targeting aims, the study and progress of drug delivery strategies to cross the BBB are supposed to be widely addressed. Above a wide overview on the most interesting and recent applications of nanomedicines to the CNS targeting, in this talk, the most recent works on poly-lactide-co-glycolide and other polymer-based NPs differently modified for BBB crossing will be reviewed. In particular, different strategies based on different ligands for BBB crossing, as exogenous-like peptides, endogenous-like peptides BBB-receptor antibodies and glyco-peptides will be detailed. In vivo and in vitro results will be commented to underline which mechanism is responsible for BBB crossing, which pathways are exploited for cell entry and specific accumulation-tropism in brain areas and even in cell type are present, dependently on type of ligands. With this talk, we will therefore try to draw an overview of the main advantages of the use of nanomedicine-based approach for innovation in crossing the most "defensive" barrier in our body, with particular relevance to neurodegenerative diseases. Besides these aspects, a critical analysis on the main causes that slow the application of nanomedicine to brain disorders will be discussed along with the identification of possible solutions and possible interventions. Moreover, a short overview of recently started IMI2 project (IM2PACT) will be described to show the tendency of both academic and industrial research in terms of novel ways and strategies for BBB crossing and to try to answer to a pivotal question: will there be a future for nanomedicine for brain diseases application and more generally for targeted nanomedicines?

MicroRNA-124-3p-enriched Small Extracellular Vesicles As a Promising Therapeutic Approach for Parkinson's Disease

Liliana Bernardino

University of Beira Interior, Portugal

Abstract:

Parkinson's disease (PD), a neurodegenerative disease characterized by the loss of dopaminergic neurons in the substantia nigra (SN), does not yet have an effective cure available. MicroRNA-124 (miR-124) has been regarded as a novel therapeutic entity for PD due to its pro-neurogenic and neuroprotective roles. However, its efficient delivery to the brain remains challenging. Previously, we have developed polymeric nanoparticles to deliver miR-124 in the brain. Here, we used umbilical cord blood

mononuclear cell-derived small extracellular vesicles as a biological vehicle to deliver miR-124 (miR-124 sEVs) to the brain, and its therapeutic effects were then evaluated in a 6-hydroxydopamine (6-OHDA) mouse model of PD. *In vitro*, miR-124 sEVs induced neurogenesis in subventricular zone (SVZ) neural stem cell cultures and protected N27 cells against 6-OHDA-induced toxicity. *In vivo*, intracerebroventricularly administered sEVs were found in the SVZ lining the lateral ventricles, striatum, and SN, the brain regions most affected by PD.

Most importantly, although miR-124 sEVs did not increase the number of new neurons in the 6-OHDA-lesioned striatum, our formulation protected dopaminergic neurons in the SN and striatal fibers, which consequently ameliorated PD-related motor symptoms. Thus, our findings support the use of sEVs as delivery agents for therapeutic miRs in the context of PD and, eventually, in other degenerative diseases. Furthermore, this works contributes to compare the therapeutic effects afforded by polymeric nanoparticles versus small extracellular vesicles in PD.

DNA-Scaffolded Nanoreactors for Biomimetic Catalysis and Molecular Sensing

Jinglin Fu

Rutgers University-Camden, NJ, USA

Abstract:

Cellular functions rely on a series of organized and regulated multienzyme cascade reactions. The catalytic efficiency of multienzyme complexes depends on the spatial organization of composite components which are precisely controlled to facilitate substrate transport and regulate activities. If these cellular mechanisms can be mimicked and translated to a non-living artificial system, it can be useful in a broad range of applications that will bring significant scientific and economic impact. Self-assembled DNA nanostructures are promising to organize biomolecular components into prescribed, multi-dimensional patterns. Here, we described a robust strategy for DNA-scaffolded assembly and confinement of biochemical reactions. DNA nanostructures are exploited to organize spatial arrangements of multienzyme cascades with control over their relative distance, substrate diffusion paths, compartmentalization and functional actuation. The combination of addressable DNA assembly and multienzyme cascades promises to deliver breakthroughs toward the engineering of novel biomimetic reactors, which have great potential for broad applications from chemical synthesis, functional biomaterials and biofuel production to therapeutics and diagnosis.

Development of DNA Education Modules for Middle School, High School, and Undergraduate Students and Educators

Michael W Hudoba

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Abstract:

DNA origami is a rapidly growing technique that enables researchers to create nanostructures with unprecedented geometric precision and is advancing molecular sensing, robotics, and nanomedicine. Due to the complexity of design, cost of materials, and cost of equipment, experiments with DNA origami have been limited mainly to graduate level laboratories at institutions that possess faculty members with expertise in the area and the financial means for expensive material and equipment. We believe that by removing some of the complexity of the design process and the hefty costs associated with DNA origami, valuable educational milestones can be achieved by young students in fields such as cellular biomechanics, biological engineering, medicine, and materials science. Introducing students to these areas of science also have the potential to advance each respective field due to increased interest and involvement by young students, who may otherwise have chosen different education and career paths.

Traditionally, nanodevices developed with DNA origami are designed using the CAD software caDNAno and fabricated following a protocol that requires the use of buffers at precise molarities (which can be expensive and require experience to create), the use of expensive specialized equipment such as thermocyclers, and a folding reaction that occurs over the timeframe of days.

This work explores the optimization of four modules, with a focus on affordability of materials and lab equipment, timing, ease of implementation by teachers and instructors, and student understanding of the procedure and its background content.

Quantification of DNA Damage Induced Repair Focus Formation via dSTORM Localization Microscopy

Varga Dániel

University of Szeged, Hungary

Abstract:

DNA double-strand breaks (DSBs) are one of the most deleterious lesions in the cells. In response to environmental stresses, cells have developed repair mechanisms to eliminate the DSBs. Upon DSB induction, several factors play roles in chromatin relaxation by catalysing the appropriate histone posttranslational modification (PTM) steps, therefore promoting the access of the repair factors to the DSBs. Among these PTMs, the phosphorylation of the histone variant H2AX at its Ser139 residue (also known as γ H2AX) could be observed at the break sites. A repair focus is made up of nanofoci. Such a substructure of repair foci can only be resolved and detected with super-resolution microscopy. Our aim was to develop a quantitative approach to analyze these γ H2AX foci by super-resolution dSTORM microscopy. The localization of individual fluorophores opened the way to quantify these proteins. However, the determination of the exact number of γ H2AX containing nucleosomes is challenging because of the stochastic nature of organic dyes during the measurements. We have established a specific dSTORM measurement process by developing a new analytical algorithm for gaining quantitative information about γ H2AX enriched repair foci. Determination of the average localization numbers in an single target molecule was one of the key steps of quantitative dSTORM. Extracting the size and the density distributions of γ H2AX foci from the measurement files was another important step of the evaluation. Our method uses the measurement files directly and does not require calibration measurements. This approach is simple and user friendly, which does not increase the measurement time.

Multifunctional Stimuli-Responsive Systems for Sensing and Therapy

Helena Iuele

CNR NANOTEC Institute of Nanotechnology, Italy

Abstract:

Material science and materials customization helped overcoming many biological issues. Sensing materials are particularly relevant for the *in-situ* monitoring of 3D cellular microenvironment alterations occurring both during physiological processes, such as tissue regeneration, and pathological processes, such as cancer evolution while therapy materials allow to treat targeted cells with one or more contextual therapies controlling and modulating their duration in space and time.

Herein, the synthesis and functionalization of materials with advanced properties will be described with a special focus on the properties they could offer for the aforementioned biomedical applications.

Optical ratiometric micro-sensors designed to track spatio-temporal pH changes of the local cellular microenvironment are presented as example of sensing materials, in particular: (i) Capsules-based biosensors placed in mesenchymal stromal cell 3D scaffolds, and (i) Highly sensitive silica-based biosensors tested with human colorectal carcinoma cells.

Electrospun composite nanofibers are presented as example of therapy and drug delivery platforms, in particular: *(ii)* gum arabic ECM-like nanofibers as platforms for *in vitro* cell growth and anticancer nanomedicine delivery, and *(ii)* magnetic nanofibers as manipulative hyperthermia material and switchable drug release platforms.

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

Nano-pharmaceuticals: A Transformative Way for Cancer Treatments

Murali M. Yallapu

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Abstract:

The United States Food and Drug Administration has permitted number of therapeutic agents for cancer treatment. Most of them have some degree of systemic toxicity which makes overbearing in clinical settings. Additionally, drug resistance, metastasis, and recurrence remain to be inexplicable in cancer therapeutics. Therefore, an urgent and unmet clinical need to deploy successful delivery nanomedicine of the approved chemotherapy agents precisely to tumors for the effective management of cancer therapy. This talk provides distinct biological and physiological characteristics of such nanomedicine. This talk will also outline specific targeted molecular mechanism(s) of nanomedicine that are responsible for enhanced anti-cancer, antimetastasis, anti-angiogenesis, and chemo-/ radiation sensitizer actions. At the end, it will be covered most recent development, proof, and applications of various nanomedicines and its effective translational approaches.

Cancer Nanotechnology: Determining the Effect of Nano-based Therapeutics in Cancer Cells vs. Normal Cells

Devika Chithrani

University of Victoria, Canada

Abstract:

One of the major issues in cancer radiotherapy (RT) is the normal tissue toxicity. Introduction of radiosensitizers such as gold nanoparticles (GNPs) into cancer cells to enhance the local RT dose has been tested successfully. However, it is not yet known how GNPs interact with other stromal cells such as normal fibroblasts (FBs) and cancer associated fibroblasts (CAFs) within the tumor microenvironment (TME). To fully elucidate the GNP-mediated therapeutic in RT, we used FBs and CAFs along with HeLa (our cancer cell line) to evaluate the differences in GNP uptake and resulting radiation induced damage. Both cancer associated cell lines had higher GNP uptake compared to FBs. This translated to higher DNA damage in CAFs (13.5%) and HeLa (9.8%) compared to FBs (8.8%). However, irradiated CAFs with GNPs did not show an appreciable difference in cell growth over time while the other cell lines did, showcasing the complexity added to GNP-mediated dose enhancement in the TME by the addition of CAFs. Therefore, our study unveils the importance of determining the NP uptake and resulting treatment outcomes not only in tumour cells but also in stromal cells within TME in understanding and improving future cancer nanomedicine.

New Multi Dimensional AFM modes to Identify Cells Using Machine Learning

Igor Sokolov

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Abstract:

New multi dimensional AFM modalities, sub- resonance tapping, Ringing mode, FT-NanoDMA allow collecting multiple images of a sample surface simultaneously. These images represent different physical/chemical information on the sample surface. As a result, it becomes possible to combine these images to identify different materials by their surface features. For example, Ringing mode, in combination with PeakForce QNM sub-resonance tapping presently allows for simultaneous obtaining 14 maps/images of different physical and chemical properties of the sample surface. FT-NanoDMA allows simultaneous recording of more than 20 dynamical mechanical parameters. This wealth of information requires special methods of data processing. Machine learning seems to be a natural method of classification of sets of complex images.

In this talk, I will describe our solution to adapt AFM imaging for use together with machine learning. The key is in a substantial reduction of the dimension of the data space by using so-called surface parameters. The Ringing

mode images of adhesion and height are used to detect the cells coming from urine of bladder cancer patients. The reduction of the imaging data space to the space of the surface parameter will be demonstrated. The steps to produce sufficient statistics using bootstrap methods will be overviewed. An important problem of overtraining will be discussed. The described method can be applied to the classification of virtually any surface, not necessarily the medical one.

Nanotechnology-based Tools for Glioblastoma and Secondary Brain Cancers

Shanta Dhar

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Abstract:

Patients with common solid tumors such as breast and lung cancers often show secondary brain metastases, which are a major cause of morbidity and mortality. Up to 40% of all patients with such a primary tumor will develop a secondary brain cancer, and these metastases in the central nervous system affect survival, neurocognition, speech, coordination, behaviors, and the overall quality of life in these patient populations. The primary treatment options for metastatic brain tumor include whole brain radiotherapy (WBRT), stereotactic radiosurgery, surgery, and chemotherapy. However, WBRT does not result in any significant improvement in quality of life, and there is only a 3- to 6-month median survival following WBRT due to progression of disease. Glioblastoma multiforme (GBM) is the most common glioma in adults which represents an aggressive brain tumor of astrocytic/neural stem cell origin. Despite the standard therapy that includes surgery followed by radiotherapy or a combination therapy, the prognosis remains poor for patients. Most chemotherapeutic options cannot be used under the settings of brain metastases or GBM due to their inability to cross the blood brain barrier (BBB). In my talk, I will discuss our strategies to deliver therapeutics to the brain to alter metabolic plasticity and adaptability in cancer cells and cancer stem cells for therapeutic gain.

Using Transferrable Graphene-based Membranes for Spatial and Temporal Control of Cell Cultures

Keith Whitener

U.S. Naval Research Laboratory, D.C., USA

Abstract:

Exerting spatial and temporal control over cell populations is a powerful capability which offers the promise of manipulating and interrogating living systems for use in advanced biological engineering such as bottom-up tissue engineering. To this end, we have developed techniques for reversibly transferring graphene-based thin film materials in a biocompatible way. Using single-layer hydrogenated graphene as well as partially reduced graphene oxide as mechanical support layers, we can deposit spatially patterned materials such as metallic electrical contacts, molecules with biochemical activity, and polymers, and transfer them to arbitrary surfaces using simple water delamination. We found that incorporating a thin gelatin layer onto the film mitigates cytotoxicity and cytolysis associated with graphene-based materials and enables transfer of materials-patterned thin films to mesenchymal stem cells without sacrificing viability. In addition, the low melting point of gelatin enables facile removal of these thin films. Simple and fast fabrication, deposition, and removal of patterned materials on cells allows for spatial as well as temporal control over external stimulus delivery to those cells. We also found that the partially reduced graphene oxide thin films are impermeable to most molecules, and we are exploiting this property along with transferrable photolithography to construct cell masks for spatially patterned biomolecule delivery and cell cocultures.

Small Molecule-based EGFR Targeting of Biodegradable Nanoparticles Containing Temozolomide and Cy5 Dye for Greatly Enhanced Image-guided Glioblastoma Therapy

Rebecca R. Schmitt

University at Buffalo, NY, USA

Abstract:

Current treatment for glioblastoma multiform (GBM) is insufficient, only affording patients an average survival time of 40 to 50 weeks. While targeted nanotherapeutics have shown promise in improving GBM treatment, tradi-

tional antibody-based targeting poses many challenges for central nervous system applications such as limited blood brain barrier (BBB) permeability and tumor penetration. To overcome these obstacles, we developed a multimodal nanoformulation which, instead, utilizes a unique small molecule targeting agent, CFMQ. In this formulation, CFMQ is coupled to biocompatible chitosan coated poly(lactic-co-glycolic) acid nanoparticles that encapsulate the chemotherapeutic agent, temozolomide (TMZ), and the NIR dye, Cy5. These targeted nanoparticles enhance cellular uptake and show rapid BBB permeability in-vitro, demonstrating the ability to effectively deliver their load to tumor cells. Encapsulation of TMZ decreases the IC50 ~17-fold compared to free drug, while co-encapsulation of Cy5 enables optical image guided therapy. Additionally, CFMQ synergistically suppresses tumor cell progression, drastically reducing colony formation (98%), cell migration (84%), and cell invasion (77%) in-vitro. Overall, this biocompatible multimodal nanoformulation exhibits an excellent therapeutic effect with high potential for image-guided, localized and controlled drug delivery of TMZ to GBM tumor cells. Our study thus has important implications for the development of nanotherapeutics for targeted drug delivery and therapy of GBM.

Cannabinoids in Tears: Novel Biomarker for Forensic Use

Denise A Valenti

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Abstract:

There are 15 states that allow for legal adult use marijuana/THC and 35 states allow medicinal use. THC is not an easy drug to measure. The most common biological matrix utilized in criminal cases for detection of cannabinoids is blood. If a driver refuses it can take up to four hours to get a court order to obtain blood. By then the active form of marijuana, THC has dissipated and the only form identifiable are the inactive metabolites of THC. Alternatives that are easy to obtain roadside are needed.

THC was found in tears using HPLC-MS/MS.

Marijuana related driving impairment presents a challenge to law enforcement as well as to the court systems. There are tests of saliva available and breathalyzers are under development. Both are problematic in that saliva does not reliably identify marijuana use from edibles and it probable that breath cannot identify edible use at all. Obtaining a sample of breath roadside is proving to be problematic.

Tears are a reasonable option. Tears have already been demonstrated as biomarkers of disease, pregnancy status and nutrient levels such as Vitamin D. Saliva and breath do not adhere/hold THC well as THC is hydrophobic and lipophilic. This is likely the reason for such poor detection with edibles. However, tears are dense with lipids and thus THC adheres strongly within the multiple layers of tears. Obtaining a tear sample with enough THC in it is simple and unlike breath, requires little post retrieval processing prior to analysis by HPLC-MS/MS.

The Role of IP in Nanotechnology Innovation

Monica Patel

Keltie LLP, United Kingdom

Abstract:

The global nanotechnology market was valued at USD 1.76 billion in 2020, and is projected to reach USD 33.63 billion by 2030, registering a compound annual growth rate of 36.4% from 2021 to 2030 [1]. Of course, there are applications of nanotechnology across a huge range of sectors, thereby impacting several global markets and fostering economic growth. For example, some of the newest innovations in the world of nanomaterials have led to significant advancements in energy conversion and storage, quantum computing, nanomedicine, and aerospace. In addition, use of computational tools, such as machine learning, is growing rapidly in aspiring to optimise nanostructures and predict improved materials.

Direct outputs such as scientific publications and patents help to assess the impact of investing in such tools and nanotechnology R&D. Several studies to date link a company's ownership of IP rights positively to its economic performance, underlining the importance of making it easier for companies to protect their innovations with IP rights [2]. In this talk, we will explore benefits of patenting in driving nanotechnology innovation and commercial-

ising inventions in this field. In addition, we will discuss specific examples of patented inventions in nanotechnology and the legal protection provided by patents and registered designs. Furthermore, we will review the hurdles to patentability, particular challenges in this field and prospects on how to overcome them.

References:

- 1. Nanotechnology Market: Global Opportunity Analysis and Industry Forecast, 2021-2030, Allied Market Research, July 2021.
- 2. Intellectual Property Rights and Firm Performance in the European Union, Firm-Level Analysis Report, February 2021.

Investigating Factors Influencing Consumer Willingness-to-pay for Nanopesticides

Peiyuan Liu

University of California, CA, USA

Abstract:

Achieving global food security requires pesticides use due to crop losses caused by pests, weeds and pathogens. As conventional chemical pesticides have induced pathogen resistance and detrimental risks to people and the environment, nanopesticides have become a unique potential alternative with higher efficiency and lower environmental impacts. However, huge knowledge gaps exist in the socio-economic aspects of their applications, particularly regarding consumer (user) willingness-to-pay (WTP) for nanopesticides. Thus, we conducted a regional survey across China to investigate factors influencing pesticide users WTP for nanopesticides, using the interval regression model and robustness test. We found that most pesticide users (97.4%) were willing to pay for nanopesticides, with a price from 25% to 40% higher than for conventional pesticides. Experience with applying pesticides, responder income, familiarity with nanopesticides, attitude toward future development of nanopesticides, and trust in industries were significant determinants of WTP. Our findings provide valuable guidance for industries and governments to develop and regulate nanopesticides in the future, contributing to crop yield improvement and sustainable agriculture.

Nano Electronics

Integrated Electrical System Based AD5933 Impedance Analyzer: Towards Multi-Selective Detection of Complex Gas Mixtures in IoT Micro-Systems

Bilel Hafsi

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Abstract:

In this paper, we present the development of miniaturized, multiplexed, and connected impedance spectrometer platform. Designed for portable measurements and adapted to wireless network architectures, our platform has been tested and realized to be used for multi-selective chemically sensitive nodes. Our designed circuit is built from low cost and low power consumption microelectronics components that achieves long duration operability without compromising on sensors measurement accuracy and precision. We used the well-known impedance network analyzer AD59331 (Analog Devices, Norwood, MA, USA) chip which can measure impedance spectra in the range 5 Hz to 100 kHz. The proposed system uses ATmega328P Microcontroller to control the AD5933 through its I2C interface and two multiplexer components ADG1608 used for calibration and data feedback. Our platform is able to interface up to 15 conductimetric chemosensors2 at the same time with the possibility to relay the information through the network for data analysis and storage.

The paper describes the microelectronics design, the impedance response over time, the measurement sensitivity and accuracy and the testing of the platform for portable conductimetric chemosensors for applications such as air quality sensing and environmental monitoring.



Figure: Printed circuit board of our compact sensing Platform based AD5933 Impedance analyzer.

Soft Nanomaterials as Plasmonic Systems

Brigita Rozic

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Abstract:

In the last years, attention has been paid to the gold nanorods (GNRs) due to their unique shape-dependent properties such as multiple plasmon bands that can be separately activated by incident light polarization. However, for the maximum efficiency of a device based on the excitation of the GNRs localized surface plasmon resonance (LSPR), GNRs need to be well aligned. We show that the use of oriented linear arrays of smectic A defects, the so-called oily streaks, enables the orientation of GNRs for a large range of diameters and for various ligands. Moreover, for the small GNRs it enables oriented end-to-end small chains of GNRs. We have characterized the orientation of single GNRs by spectrophotometry and Two-Photon Luminescence (TPL).

Combining plasmonic absorption measurements, TPL measurements and simulation of the plasmonic absorption, we show that the end-to-end GNR chains are either dimers, trimers or quadrimers, all parallel to each other. A motion of the GNRs along the dislocations appears as a necessary ingredient for the formation of end-to-end GNR chains, the gap value being driven by the balance between the attracting Van der Waals interactions and the steric repulsion between the GNRs and leading to interdigitation of the neighboring ligands. We thus obtained electromagnetic coupling of nanorods, demonstrate it through light polarization.

Sensitive Interferometric Plasmon Ruler Based on a Single Nanodimer

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Abstract:

The plasmon ruler has attracted considerable attention for measuring the nanoscale distance between two plasmonic nanoparticles (NPs) e.g. to measure the bending of single DNA-strands. The conventional plasmon ruler relies on the spectral shift of the surface plasmon resonance (SPR) of the dimer which is caused by the distance-dependent dipole–dipole coupling. By detecting the phase shift of the scattered signal, the same spectral information can be obtained. By combining a confocal microscope and a Michelson interferometer we are able to measure the phase change caused by a single nanoparticle in a diffraction-limited focal spot. The respective plasmon ruler is realized by a gold nanoparticle dimer (GND) deposited on a flexible polydimethylsiloxane substrate, that allows us to vary the gap between the GNDs by stretching of the substrate and record the phase shift as a function of the changing gap-width. Interestingly, an increase of the gap by 11 nm leads to a considerable phase shift of 94°, even though it is only associated with a 11 nm spectral shift of the SPR. We find that both the spectral and phase shifts have the same r^{-3} dependence on the particle gap as expected for dipole–dipole coupling.

Octahedral Distortion Driven by CsPbI3 Nanocrystals Reaction Temperature – The Effects on Phase Stability and Beyond

Paola Vivo

Tampere University, Finland

Abstract:

Cesium lead iodide (CsPbI₃) perovskite nanocrystals (NCs) suffer from a known transformation at room temperature from their red-emitting (black) to non-emitting (yellow) phase, induced by the tilting of PbI₆ octahedra. While the reported attempts to stabilize CsPbI₃ NCs mainly involve Pb²⁺-site doping as well as compositional and/ or NC surface engineering, the black phase stability in relation only to the variation of the reaction temperature of CsPbI₃ NCs is surprisingly overlooked. We report a holistic study of the phase stability of CsPbI₃ NCs, encompassing dispersions, films, and even devices by tuning the hot-injection temperature between 120–170 °C. Our findings suggest that the transition from the black to the yellow phase occurs after over a month for NCs synthesized at 150 °C (150@NCs). Structural refinement studies attribute the enhanced stability of 150@NCs to their observed lowest octahedral distortion. The 150@NCs also lead to stable unencapsulated solar cells with unchanged performance upon 26 days of shelf storage in dry air. Our study underlines the importance of scrutinizing synthesis parameters for designing stable perovskite NCs towards long-lasting optoelectronic devices.

New and Emerging Van der Waals Semiconductors for Electronic and Photonic Applications

Moh R. Amer

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Abstract:

Van der Waals semiconductors are special materials that have grasped the attention of research communities. 2-Dimensional materials such as graphene, black phosphorus, and transition metal dichalcogenides have been under investigations for device applications. Yet, to this date, there are numerous unknowns surrounding devices fabricated using these materials, which prompts wide investigations into electronic and photonic device operations. In this talk, I will show our recent work on nanodevices fabricated using 2D materials. I will show our recent methods to fabricate 2D materials with improved electrical characteristics by introducing our pulsed thermal annealing method. I will also demonstrate our recent investigations on emerging 2D materials such as Hafnium Diselenide (HfSe₂) and Germanium Sulfide (GeS) and how their electrical conductivity can be altered using laser induced methods and 2D deposition, respectively. I will also discuss our recent optical findings on 2D Zirconium based materials where observed Raman peaks can be completely different for the same nanosheet. These Raman peaks have been found to depend on the crystallinity of the material. Finally, I will discuss our recent demonstration of tunable light emission from treated black phosphorus nanosheets where the emission tunability has a wide bandwidth of 110nm. The origin of this tunable light emission is found to be caused by the formation of black phosphorus oxide which exhibit a direct band gap in the range of the tunable emission. Our investigations provide a potential platform of 2D nanodevices for future electronic and photonic devices.

Thickness and Spin Dependence of Raman Modes in 2D Magnet Fe₃GeTe₂

Liangbo Liang

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Abstract:

Two-dimensional (2D) layered magnetic materials have attracted increasing attention after the 2D ferromagnetic order was first discovered in chromium compounds such as CrI_3 and $Cr_2Ge_2Te_6$. The family of 2D magnets contin-

ues to grow larger and larger: in addition to insulating CrI_3 and $Cr_2Ge_2Te_6$, Fe_3GeTe_2 as a 2D magnetic metal has also joined the family. The outstanding physical properties in Fe_3GeTe_2 demonstrate its potential values in fundamental research and future applications. Before any practical applications of 2D magnets, the lattice vibrations (i.e., phonons), the magnetic orders (i.e., spins), and their coupling need to be understood first. Raman spectroscopy is among the most fast and reliable experimental techniques that can probe both phonons and spins in 2D magnetic materials. To explain and guide experimental Raman measurements, first-principles modeling of Raman scattering based on density functional theory (DFT) is often required. Here, I will highlight a recent Raman modeling-driven project on Fe_3GeTe_2 . Its phonon vibrations and Raman intensities were calculated from the bulk to the monolayer. The spin-phonon coupling effect was investigated by considering different interlayer magnetic orders: ferromagnetic and antiferromagnetic. The frequencies of Raman modes in Fe_3GeTe_2 were found to exhibit considerable dependence on both the layer number and spin order. The results not only reveal the notable spin-phonon interactions in Fe_3GeTe_2 , but also demonstrate that Raman modes can be utilized for characterizing the sample thickness and interlayer magnetic order in Fe_3GeTe_2 .

Design and Simulation of Fundamental Building Blocks for All-Optical Computers (Universal Gates Only)

Saif Hasan Abdulnabi

Imam Ja'afar Alsadiq University, Iraq

Abstract:

Though photonics displays an attractive solution to the speed limitation of electronics, decreasing the size of bulky photonic components is one of the major problems with the implementation of photonic integrated circuits that are regarded the challenges to produce all-optical computers. Plasmonic can solve these problems, it be a potential solution to fill the gaps in the electronics (large bandwidth and ultra-high speed) and photonics (diffraction limit due to miniaturization size). In this paper, Nano-rings Insulator-Metal-Insulator (IMI) plasmonic waveguides has been used to propose, design, simulate, and perform all-optical universal logic gates (NOR and NAND gates). By using COMSOL Multiphysics (version 5.5), the structure of the proposed plasmonic universal logic gates are designed and numerically simulated by two dimensions (2-D) structure. The materials of the proposed structure are silver and Glass. The operation principle of this device is based on the constructive and destructive interferences between the input signal(s) and control signal. The performance of the proposed device is measured by three criteria; the transmission, extension ratio, and modulation depth. Numerical simulations show that a transmission threshold (0.3) which allows achieving the proposed plasmonic universal logic gates in one structure at 1550 nm operating wavelength. However, in single state, the transmission of the proposed plasmonic NAND gate exceeds 100%, that is (130.6%). Furthermore, the proposed structure are designed with a very small area (400 nm × 400 nm). In the future, this device will be the gateway to the photonic integrated circuits and it has regarded fundamental building blocks for all-optical computers.

Active Polymer: Perovskite Nanocrystals Blends as Possible Active Materials for Photonics and Optoelectronics Devices

Marco Anni

Università del Salento, Italy

Abstract:

The combination of lead halide perovskites nanocrystals (NCs) and conjugated polymer in a blend film opens the way to the realization of hybrid active layers with widely tunable optical and electrical properties, able to combine the best properties of both families. We investigated the emission properties of different polymer:perovskite NCs blends, evidencing that these hybrid films show photoluminescence spectra made by the linear superposition of the spectra of the components. This feature opens the way to the use of these blends as light emitting systems with broadly tunable emission color, including white emission. Moreover we investigated the interaction between the polymeric and the perovskite component, mainly unexplored to date, of a poly(9,9-dioctylfluorene-co-benzothiadiazole)(F8BT):CsPbI1:5Br1:5 nanocrystals hybrid film. We demonstrate that the primary interaction channel is charge transfer, both from F8BT to the NCs and from the NCs to F8BT, while Förster Resonant Energy Transfer has not visible effects, despite the excellent spectral overlap between F8BT emission and NCs absorption. Moreover we show that the charge transfer is assisted by energy migration within the F8BT excited states distribution and that it is dependent on the local micromorphology of the film. The possible relevance of our results for the development of hybrid organic-perovskite optoelectronic devices will be discussed.

Plasmonic Nanoresonators Embedded into Active Shells Optimized for Near-field and Far-field Stimulated Emission

Maria Csete

University of Szeged, Hungary

Abstract:

The coexistence of loss and gain results in rich nanophotonical phenomena in light-generating systems. Configurations of spherical plasmonic nanoresonators with dielectric-gold-gain (DMG) and gain-gold-gain (GMG) composition were optimized to maximize the stimulated emission in the near-field (NF-c), the farfield outcoupling (FF-c) and to achieve spasing (NF-c^{*}). Numerical pump and probe study was performed to extract the S-curves, optical responses and cross-sections, near-field and far-field spectra, polar angle distribution of radiation, and to inspect the effect of Rh800 dye concentration. At moderate concentration GMG outperforms the DMG composition considering the smaller lasing and gain thresholds, larger slope efficiency, averaged probe-field enhancement and spectral peaks at a specific pump. In GMG-NF-c the optical cross-sections are larger. GMG-FF-c possesses smaller power-outflow threshold and additional zero-crossing in the extinction cross-section. The GMG-NF(FF)-c composition enables more pronounced near-field bandwidth narrowing and larger internal (internal and external) quantum efficiency. By increasing the concentration, the zero-crossing in extinction cross-section proves entering into the spasing regime in both nanoresonators, which is facilitated by time-competing dipolar and quadrupolar modes, and the power is transferred into the far-field more uniformly. The GMG-NF-c* possesses smaller lasing, gain, power-outflow and optical cross-section thresholds. For GMG-NF-c* the slope efficiency is larger, the averaged near-field enhancement at the probe wavelength is larger, the near-field bandwidth narrowing is more pronounced and the quantum efficiency is larger. The extrema emerge at a smaller pump in the local E-field, absorptance, and optical cross-sections in GMG-NF-c*. Based on this gain-metal-gain composition is proposed for lasing and spasing operation.

Enhancement of THz Detection by Using an Asymmetric-Dual-Grating-Gate Graphene FET

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Abstract:

The unique optical and electronic properties of graphene based heterostructures open the way for the development of new graphene-based devices. Indeed, new hybrid graphene-based devices operating in the terahertz (THz) range are appealing since it is one of the least explored frequency regions and their applications hold potential to revolutionize different fields like security, medical imaging, or high-speed wireless communication. In this work, we report on an enhancement of the detection of terahertz radiation by using a graphene-based FETs with asymmetric dual grating gates (ADGG-GFET) and a few-layers thick of graphite as back gate. The device was fabricated with a stack of h-BN/Graphene/h-BN/Graphite on a standard SiO2/Si substrate (Figure (a)). The device was illuminated under 0.3 THz radiation from 4K up to room temperature and a clear photocurrent was measured while biasing with the top gate. Moreover, when a positive (or negative) voltage was applied on the few-layers graphite back-gate, we observed a clear enhancement of the measured photocurrent under illumination of the 0.3 THz radiation (Figure (b)-(c)).



Figure: Optical image of the ADGG-GFET where the graphene sheet has been highlighted with a green dashed line (a) and the THz photoresponse as a function of the Top Gate 2 (TG₂) voltage for different positive (b) and negative (c) back-gate voltages under 0.3 THz. T = 77K.

New D-A-D Systems Containing Porphyrin Cores as Electrondonors for BHJ-SMOSCs

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Universidad de Castilla-La Mancha, Spain

Abstract:

Organic solar cells (OSCs) consisting of a bulk heterojunction (BHJ) active layer are promising for the production of flexible photovoltaic devices. Inspired by photosynthesis in nature, porphyrins and their derivatives have been explored as SM donors because chlorophylls are strong chromophores and porphyrins are analogues of chlorophylls. Such molecules have been explored as donors for BHJ OSCs because they possess high absorption coefficients, and their optical and electrochemical properties can be easily tuned by functionalization of the periphery. The overall PCEs of the OSCs based on porphyrin derivatives as donors in molecules with an A-D-A configuration have been significantly improved through molecular design.

The structure A-D-A have been the most studied while the search of D-A-D chromophores is not widespread and only few examples have been reported to date. Therefore, there is a lack of comparative studies between A-D-A and D-A-D to understand how the alteration of the molecular backbone influence the properties of the molecules and the efficiency of devices.

In this communication, we present the synthesis and the studies of the electronic properties new D-A-D systems based on Zn-porphyrins and diketopyrrolopyrrole (DPP).

Optimization of Silver Chalcogenide Quantum Dots for NIR-II Potodetectors

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Abstract:

Silver chalcogenide colloidal quantum dots (QDs) can absorb and emit at wavelengths in the second near infrared window (NIR-II, 1000–1700 nm), which enables them to be an excellent candidate as an infrared nanomaterial, with a variety of potential applications, including bioimaging, biosensing, quality control, and machine vision. During Ag₂Se synthesis in organic solvents, accurate size (mean diameter 3.7 nm) control of Ag₂Se nanocrystals with a distinct excitonic absorption peak and a good particle yield was achieved by employing secondary phosphine (as nucleating agent) to elevate the precursor reactivity. By incorporating a suitable hole-transporting layer between the active layer and Ag anode, the resulting photodiode structured photodetectors showed a responsivity of 4.17 mA/W at 1200 nm and an EQE of over 1% at 1150 nm. During Ag_2 Te synthesis in organic solvents, a number of synthetic parameters including Ag-to-Te feed ratios, secondary phosphines, and ligands, etc. play a critical role in determining the Ag_2 Te QD quality, as measured by the size and size distribution, colloidal stability, photoluminescence quantum yield (PL QY), and the particle yield. After optimization of synthetic parameters, relatively large Ag_2 Te QDs with distinct excitonic absorption peaks (> 1000 nm) and good PL QYs (up to 6.2%) were obtained. The synthesized Ag_2 Te QDs application in NIR-II photodetection has been demonstrated with a responsivity of ~1.5 mA/W at 1400 nm. Such a combination of optimized quantum dots and device performance demonstrates that silver chalcogenide QDs offer a low-toxicity route for low-cost fabrication of NIR-II photodiodes.

Nanomaterial Design for Solar Driven Water Desalination

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Abstract:

Solar energy is considered as the most abundant renewable energy source. Conventional solar desalination technology uses the sun light and/or concentrated sun light to heat the bulk liquid for generation of water steam, which has relatively low solar vapor conversion efficiency (30%-50%). New design strategies of materials and structures based on localized energy absorbing and heating can significantly increase the solar vapor conversion efficiency (>90%). In this talk, I report our recent work on design of materials and structures for efficient solar-driven water desalination. Inspired by the high efficiency of vapor transpiration of a leaf, we demonstrate a leaf-biomimetic material structure for a solar still with the solar vapor generation efficiency beyond 100% and the total production rate of 3.09 kg·m⁻² ·h⁻¹ under one sun irradiation. The leaf-inspired 3D material structure has a hydrophilic polyvinyl alcohol (PVA) foam layer (equivalence to the mesophyll tissue layer in a leaf) with high porosity and low thermal conductivity, a photothermal polypyrrole layer (equivalence to the chlorophyll layer in a leaf). The prototype solar still demonstrates desalination and purification of brine and seawater continuously under the nature sunlight for 12 hours. Additionally, we designed and built portable solar stills based on carbon black coated fabrics and evaluated their performance under the nature sun light as well as the quality of the purified water.

Metalloid Group 11 Clusters: Novel Structures and Properties

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Abstract:

Metalloid clusters of the general formula $M_n R_m$ with n > m (M = Al, Au, Ag etc.; R = substituent) are ideal model compounds to shed light onto the nanoscaled area between molecules and the solid state on an atomic level. In case of gold the structural characterization of the multishell metalloid gold cluster $Au_{102}(p-MBA)_{44}$ (p-MBA = para-mercaptobenzoic acid) was a breakthrough in this field indicating some important aspects for such cluster compounds like the importance of the staple motive in the ligand shell. Lately we could show that also other structural motives can be realized within nanoscaled metalloid gold clusters whereby Au_4S_4 rings within $Au_{108}S_{24}(PPh_3)_{26}$ is only one example.^[3] Here we describe further examples in this field together with investigations on the physical properties of the cluster arrangement in the solid state, showing that beside novel structural motives also novel properties are realized for such nanoscaled clusters opening the door for a variety of future applications.



Figure: Molecular structure of the metalloid gold cluster $Au_{108}S_{24}(PPh_3)_{26}$. The arrangement of the different shells is highlighted by a polyhedral presentation.

Green Synthesized Nanomaterials for Diverse Applications

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Abstract:

Nowadays scientific community is majorly concerned with new challenges present in health and environmental areas. In this way, nanotechnology holds a great potential towards applications of nanoparticles in many ways, including novel fields of science and technology. Nanotechnology refers to a synthesis and alterations of particles smaller than 100 nm. Nanoparticles are used in medical sciences, particularly in drug delivery, imaging and diagnosis. Nanoparticles possess high surface to volume ratio due to its small size, which gives them very distinctive features. Researchers are planning to synthesize nanoparticles and design Nano devices for the future applications in the fields of medical sciences, environment, energy, information, communication, industries and also food technology.

Green synthesis, produces nanoparticles for a minimal price with gentle strain, temperature, and pH that escapes the hurtful elements for the creation. Phytonanotechnology utilizes different pieces of the plant like root, stem, seed, and leaf for the development of nanoparticles. It has been exemplified in different papers that biomolecules (proteins, nutrients), plant extracts (flavonoids, terpenoids), and microorganisms (microbes, parasites and yeast) are responsible for the green combination of various types of nanoparticles.

There is a huge need to develop better approaches utilizing green nanotechnology to expand the sufficiency of available prescriptions and antiviral/antimicrobial material. During the green synthesis of NPs, products from nature or those imitative of natural products have been used as reducing and capping agents (Figure). The methods involved are typically simple, environmentally friendly and naturally compatible one-pot processes.



Figure: Green Synthesis Mechanism

Plant extracts consist of numerous phytochemicals, such as flavonoids, phenolic acids, alkaloids, saponins, carbohydrates, amino acids and proteins, and terpenoids, that play a vital role in synthesizing NPs from metallic ions, as they act as capping/stabilizing and reducing agents. Green synthesized NPs are employed in various areas of nanomedicine, chemistry and related fields for use in drug carriers for targeted delivery, antimicrobial agents, DNA investigations, biosensors, catalysts, separation science, cancer treatment, gene treatment and magnetic resonance imaging. Plant extract based synthesis of nanoparticles makes the use of various natural products which can produce nanoparticles with more purity. Other published research reports of various forms of nanoparticles of oxide and dioxide including polymer-coated nanoparticles; Cu- nanoparticles; Au- nanoparticles; Ni and Pt-, Pd-, Si-nanoparticles; Ag- nanoparticles; CuO- nanoparticles; ZnO- nanoparticles; TiO₂- nanoparticles; ZrO₂- nanoparticles and FeO nanoparticles based on the simple plant extracts.

We have attempted to include a detailed biosynthesis detail of different metallic nanoparticles from herbal extracts. The purpose of this research was to better understand and describe the mechanisms underpinning stress resistance and NP-mediated plant tolerance enhancement via diverse biomedical applications.

On the "Super" Storage of Hydrogen in Graphite Nanofibers

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Abstract:

In this work, data of Rodriguez-Baker et al. and some others were analyzed in relation to the long-term, i.e., about 25 years, problem of "super" storage of "reversible" (at 300 K) hydrogen (\sim 38±10 wt.%, i.e. the atomic ratio (H/C) \approx 7±3)), along with "irreversible" hydrogen (\sim 11±3 wt.% ((H/C) \approx 1.5±0.4)) in activated graphite nanofibers (GNFs). For a more in-depth study of the above problem, an effective methodology of analyzing the thermal desorption spectra (TDS) of hydrogen was developed and used. Such an analysis of the reported TDS and thermogravimetric data of Rodriguez-Baker et al., relevance to the storage of "irreversible" hydrogen in GNFs, showed the presence of three desorption peaks, including the main peak #1 (\sim 8.4 wt.% ((H/C) \approx 1.1)) with the desorption activation energy of about 40 kJ/mol(H2). The physics of "super" storage of hydrogen in GNFs can be based on the hydrogen spillover effect and on the Kurdjumov phenomenon of thermoelastic phase equilibrium. There is a real opportunity to reproduce the above results on the "super" storage of "reversible" hydrogen, but only with the disclosure of the know-how of the technology of activation treatment of GNFs, which ensures the appearance in them the peak #1.

Investigation of Cellulose Nanocrystals (CNC) and Cellulose Nanofibers (CNF) as Thermal Barrier and Strengthening Agents in Pigment-Based Paper Coatings

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Abstract:

In response to food packaging improvements, this study investigates changes in mechanical and thermal barrier properties of pigment-based paper coatings when cellulose nanocrystals (CNC) and cellulose nanofibers (CNF) are added to the formulation. All coating components were able to form stable dispersions between pH 7-9 (Zeta Potential > |30 mV|) except CNF, which favored stable dispersions at higher pH. Hydrodynamic diameters (D_h) of CNC and CNF suspensions were reduced when interacting with CaCO₃ particles, however latex binder and dispersant values were unaffected by CaCO₃ concentration. Thermal barrier performance was quantified by measuring the Δ T across coated samples, with and without nanoparticle additives. Both CNC and CNF additives significantly contributed to the Δ T measured, with the best result recorded for 2 wt% CNF, pH 7, and a drying rate of 25°C/min. This sample recorded 37 ± 6 °C *higher than* the Δ T value for baseline coatings (without additive). Dynamic Mechanical Analysis (DMA) showed a higher storage modulus for all samples containing CNC and/or CNF compared with the baseline coating, suggesting a material with greater resistance to deformation from applied load. Higher dissipation energy was also observed, however lower tan delta values suggest improved mechanical properties with both additives overall.

New Optical Sensor Based on Au@MX2 Hybrid for The Detection at Low Traces

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University of Sfax, Tunisia

Abstract:

During the last decades, nano-sensing and quantifying have become a premonition worldwide. Indeed, nanomaterials bring new and fascinating features to many materials compared with their bulk counterparts. Thus, the development of several industrial gadgets is achieved such as solar cells, sensors, LEDs... Beyond graphene, several nanomaterials have been synthesized denoting metal oxides, graphene oxides, and transition metal dichalcogenides (TMDCs) materials. The later family is favored by the high carrier mobility, high surface-to-volume ratio, and bandgap tunability. Owing to these features, TMDCs materials possess a great potential for application in medicine, sensing, biology... Among these materials, molybdenum disulphide (MoS_2) is extensively studied, and since that various TMDCs materials are synthesized and studied denoting tungsten disulphide (WS_2), molybdenum diselenide ($MoSe_2$), tungsten ditelluride (WTe_2) ...

Herein, we have exfoliated MoS₂ and WS₂ NS with liquid-phase exfoliation (LPE) technique, and the exfoliated nanosheets number was determined based on Raman and UV-Vis data. Moreover, UV-Vis data was used to extract much information; concentration and mean length of MX2 NS. Furthermore, we have used both MoS, and WS, to develop nanoplasmonic semiconductor sensors through the coat of MoS₂ and WS₂ nanosheets (NS) with gold nanoparticles (AuNPs). This fact reveals the charge transfer between NPs and the semiconductor where the type of junction is defined thanks to the semiconductor theory. Since we aim at the sensing field, using AuNPs is the best choice owing to its stainless and inert. To detect at low traces, we used enhanced Raman spectroscopies (ERS) applied on the hybrid Au@MX₂ (MX₂=MoS₂, WS₂). These techniques are surface-enhanced Raman spectroscopy (SERS) and photo-induced enhanced Raman spectroscopy (PIERS) where the prior tool has an extra step compared with the first one. This step is the pre-irradiation of the substrate with UV-C light leading to the enhancement of the conventional Raman signals. A reporter molecule known as 4-mercaptobenzoic acid (MBA) is used to achieve the sensing procedure. The overall enhancement factor was in the order of 106 for both substrates. Nevertheless, the vibrational modes were improved with a factor of 4 for SERS Au@MoS₂ and ~9 for PIERS Au@WS₂ optical platforms. Regarding the enhancement origin is still unknown until now, however, scientists have proposed two effects the first is electromagnetic (EM) and the second is charge transfer (CT). The Raman signals will be boosted in the ERS techniques and strongly enhanced when the electromagnetic field E is almost |E|4 since AuNPs possess localized surface plasmon resonance (LSPR) and/or hot spots obtained after simple irradiation, The charge transfer effect was well observed in the case of PIERS Au@WS, resulted by extra electron where its density (ED =1.8%) was determined based on the pre-post UV-C irradiation spectrum. These findings prove that the Au@WS₂ sensor works well with PIERS in the detection of low traces.

Uniform Energy Deposition via Optimized Passive and Active Plasmonic Nanoresonator Distributions

Maria Csete

University of Szeged, Hungary

Abstract:

Uniform heating of targets by short laser pulses is crucial in biomedical, light harvesting and renewable energy extraction applications of plasmonic nanoresonators, moreover elimination of instabilities is a precondition of stable laser fusion. Distributions of silica-gold core-shell nanoresonators and gold nanorods were optimized in passive and active dye doped dielectric targets. The absorptance and deposited energy was increased and the uniformity of their distributions was improved using optimal plasmonic nanoresonator distributions. In passive (active) targets singlepeaked Gaussian (double-peaked) nanoresonator distributions resulted in significantly smaller standard deviations. The dye transition-time and the population inversion level in the active medium had significant impact on the energy deposition. For uniform nanoresonator distribution the energy deposited in the active target doped with dye of 2.1 ns transition-time was significantly increased compared to the analogous passive target. Whilst the

uniformity of the energy deposited in the complete target was similarly and considerably improved, the uniformity inside the core-shell nanoresonators (nanorods) was slightly (twice-more) weakened by the active medium. For smaller transition-time of 24 ps the amount of deposited energy is slightly better increased and the standard deviation of the energy distribution was twice-more reduced throughout the complete target by the active medium in case of core-shells compared to nanorods. By adjusting the distribution, the energy deposited inside target was slightly further increased and the uniformity of the deposited energy was further improved with respect to passive targets. Optimized and adjusted core-shell nanoresonator distributions are proposed to balance the energy deposited in passive and active targets.

Atomic Oxygen Exposure Effect on Electromagnetic Reflectivity of Small Satellites

Andrea Delfini

Sapienza University of Rome, Italy

Abstract:

Nowadays, aerospace research and industry is focused on the development of a novel typology of small satellites, namely cube-sat or nano-satellites, due to both the need of space mission cost saving and the emerging service capabilities envisaged by the constellations of such items. In this framework, a main feature to take into account is the satellites observability, which represents a crucial task since the low radar cross section of relatively small orbiting objects. Furthermore, the effect of the space environment on the electromagnetic behavior of the satellite outer surfaces must be deeply established in order to ensure the suite working of the spacecraft subsystems during its lifetime. In this research, different plates manufactured to be used as satellite structural panels were subjected to atomic oxygen irradiation and characterized in microwave free space set-up, with the aim to analyze the effect of an harsh space aging factor on the satellite electromagnetic signature. The electromagnetic reflectivity of advanced metallic and ceramic structures, such as titanium- and carbon/carbon-based tiles, was measured before and after atomic oxygen exposure; the performances of an in-house developed coating based on ceramic nano-particles were also investigated. The experimental results show that an addressed prototypal design of small satellite structural plates is due in order to mitigate the space environment detrimental effects on the exposed surfaces microwave reflectivity, thus avoiding systems worsening in terms of monitoring, tracking and surveillance effectiveness.

Cell-free Biosynthesis Exploiting Nanoparticle Scaffolds and Enzymatic Channeling

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Abstract:

Amongst technologies being developed for synthetic biology, cell-free approaches are becoming more prominent as they offer many advantages to address confounding issues associated with cellular systems including especially toxicity and off-pathway affects. Making these systems as simple and efficient as possible will be key to their success. From a purely minimalist perspective, multistep biosynthetic systems (i.e. enzymatic cascades) only require enzymes, their cofactors, and the substrate, however, such approaches typically suffers from reaction diffusion limitations and long-term enzyme instability. We are attempting to address these latter issues in pursuit of efficient minimalist synthetic systems by using nanoparticles (NPs) to both stabilize the enzymes and allow them to form nanoclusters that access channeled catalysis. Using semiconductor quantum dots (QDs) and the enzymes from saccharification and oxidative glycolysis as a prototypical system, we have developed methods that allow the enzymes to self-assemble with the QDs into catalytic nanoclusters. Within these systems, catalytic flux is improved by several orders of magnitude and detailed analysis along with numerical simulations show that this arises from both enzymatic stabilization and channeling phenomena. Incorporation of non-spherical QDs and optimization of relative enzymatic ratios (and catalytic rates) have also boosted efficiency dramatically. Examples of systems utilizing 10-14 enzymatic steps will be presented along with analysis of cluster formation and their channeling processes. The near and long-term potential of this approach will be discussed.

Universal Nanoscale Thermoelectric Power Generator for Energy Harvesting Applications

Faisal Alamri

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Abstract:

Layered 2-Dimensional (2D) materials have attracted the attention of researchers due to their unique and superior properties. Nevertheless, few investigations reported in the literature on Thermoelectric (TE) power generators using low dimensional materials. One major issue that TE power generators at the nanoscale suffer from is the packed design in a miniscule area, which hinders temperature gradient observation at the nanoscale. In this study, we present a universal TE power generator design for low dimensional materials and simulated the output of this TE power generator using COMSOL software. Multiple designs and geometries are tested which focused on joule heating using a metal heater. A vital requirement of our TE power generator design investigations is the maximum temperature gradient obtained across the low dimensional thermoelectric material. We show that this temperature gradient can be obtained through confinement of the metal heat electrode. We discuss the limitations of our designs and show that heat irradiated from the metal heat electrode into the substrate can impose significant challenges on the output of the power generator. Additionally, we investigate the optimal design with different environmental settings and estimate the TE power generator efficiency using Tungsten Diselenide (WSe₂) and Molybdenum Disulfide (MoS₂) as the materials of choice. Our design can be a stepping milestone towards implementing nanoscale thermoelectric power generators for energy harvesting applications.

Preparation of Graphene Nanoparticle Surface Modified Metal Oxide Doped Soda-Lime Glass Composite for Application in Water Purification

Aban Mandal

Jadavpur University, India

Abstract:

The work enumerates the production of Graphene Oxide (GO) nanoparticle surface modified Metal Oxide doped Soda-Lime Glass Composite, with excellent adsorption capacities as packed bed media for primary treatment of water, prepared following an self-assembly reaction between the colored glass containing metal oxides and GO, followed by thermal ageing of the composite. The interfacial interactions between the Soda-Lime glass surface and GO was studied using Fourier-transform infrared spectroscopy and Scanning electronic microscopy. BET analysis showed increased surface area of the composite than its precursors, study concerning zeta potential and zero-point charge depicted optimum pH sensitivity of the composite. Column-adsorption experiments were carried out in order to quantify the adsorption kinetics and adsorption capacities of the composite and compared with the precursor materials. The Soda-Lime Glass composite was evaluated for the removal of some organic dyes using UV and Visible Light spectroscopy and removal of As(V), Pb(II), Cd(II), Cr and Fe as well as hardness in water, using Inductively Coupled Plasma Optical Emission Spectroscopy, compared to the precursor, the synthesized composite exhibits higher dye removal efficiency, better adsorption capacities for heavy metals/ metal contamination as well as removal of turbidity and organic matter. This escalation is due to better synergistic molecular interactions of metal oxides in the soda lime glass, the functionalized groups in Graphene Oxide and greater surface area of the composite. These results conclude that the potential application of the composite for primary water treatment as a replacement of sand filtration.

The Developing Natural Convection Visualization of Water - Ethylene Glycol Mixture based Fe₃O₄ Nanofluids in Eccentric Annular Ducts in Low Temperature Applications

Nur Cobanoglu

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Abstract:

Rapid growth of energy demand requires passive heat transfer techniques to recover, transfer and use of generated heat to improve energy efficiency and reduce energy consumption. Since refrigeration systems compromise a large portion of the energy consumption in buildings, energy efficient solutions are proposed for vapor compression systems. Suction line heat exchangers are generally used to increase system capacity and protect the components of the vapor compression systems by subcooling the refrigerant at high-pressure side and superheating at the low-pressure side. Single-phase natural circulation loop, as passive heat transfer system, can be considered as alternative to suction line heat exchangers in vapor compression systems by locating the cooling and heating end double pipe heat exchangers in the low- and high-pressure sides of the refrigeration cycle, respectively. This study aims to numerically investigate the potential of the nanofluids as a heat transfer fluid for superheating the refrigerant at low-pressure side of the vapor compression system. Within this scope, water-ethylene glycol mixture (50:50) based Fe₃O₄ nanofluid is used as working fluid due to its advantages of higher thermal conductivity and lower viscosity values which could be considered as positive effects for passive systems. A 3D transient numerical model has been proposed to understand the developing laminar flow characteristics of the nanofluid at the low temperatures by visualization of the eccentric annular flow propagation.

A Novel Nanocomposite Coating for Flexible Food Packaging – The Effect of Dispersion Preparation and Coating Processes on the Final Oxygen Barrier Performance

Stefan Schiessl

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Abstract:

The already reported low oxygen permeability values, achieved for EVOH coatings by integration of platelet shaped silicate nanoparticles, accompany either with significant efforts in modification of the nanoparticles and/or polymer matrix, or with disproportionate expense in the coating techniques. The objective of this study is to investigate the effect of the various nanocomposite preparation and coating processes on the morphological properties and thereby, on their oxygen barrier performance. The studies on the composition optimization of an un-modified EVOH lacquer and natural abundant sodium montmorillonite (MMT) indicated that a sufficient exfoliation of MMT was achieved by ball milling in an aqueous dispersion and that no additional effort was necessary for (chemical) interaction of MMT and EVOH. An MMT concentration of 50 wt.% was found to decrease the oxygen permeability of EVOH below 0.2 cm³ [STP] µm m⁻² d⁻¹ bar⁻¹ (at 23 °C, 50 %RH), resulting in a barrier improvement factor of 12. The scaling up of the various processing stages of this coating formulation was undertaken to prove its industrial feasibility. The slot-die coating technique was successfully applied to coat the nanocomposite lacquer at different dry layer thicknesses from 1 up to 15 µm. The coatings were performed on a roll-to-roll pilot line, running stable for more than 4 h and 1000 m. These studies show the routes for a feasible large-scale production of single oxygen barrier coatings and their corresponding application in flexible food packaging.

Influence of Engineered Nanoparticles on Properties of Water in Soil Organic Matter

Marta Miklasova

Brno University of Technology, Czech Republic

Abstract:

Nowadays, engineered nanoparticles are largely used, making them a potential pollutant for the environment, including soil. Much research has been conducted on the potential adverse effects of nanoparticles on soil biota. However, the impact of nanoparticles on soil properties is not still fully understood. This work is focused on the influence of two types of 20-nm-sized titanium dioxide (TiO_2) nanoparticles (rutile, anatase) on selected water properties in soil organic matter dried at various relative humidity (43, 70, and 95 %). The study builds on previous research on platinum nanoparticles, which revealed that these nanoparticles influenced three-dimensional water structure and, consequently, water properties. Using differential scanning calorimetry (DSC), we discovered that the titanium dioxide nanoparticles reduced stability of water molecular bridges (i.e., water clusters) under 70% relative air humidity. Also, a general decrease of water evaporation enthalpy, which represents water retention of soil, was identified within measured data. Additionally, TiO₂ nanoparticles had an impact on total water in the soil. Under low relative humidity, rutile and anatase affected soil differently, probably due to their various hydrophilicity. Under higher relative humidity, this effect was insignificant due to better soil hydration. Lastly, ice melting and water evaporation enthalpies of nanoparticle solutions were studied to confirm nanoparticles' presumed effect on pure water. The ice melting enthalpy of the solutions increased compared to pure water, while the evaporation enthalpy showed a reverse trend (decrease). These conclusions confirmed that the TiO₂ nanoparticles influence pure water and soil water even at very low, environmentally relevant concentrations. That can be a potential risk to the environment. Also, TiO₂ nanoparticles contamination can increase evaportanspiration, leading to soil desiccation.

A Study of Solvent Systems for Nickel Nanopastes Used for Nanojoining

Benjamin Sattler

Chemnitz University of Technology, Germany

Abstract:

Particles of nanometer scale exhibit remarkable properties due to their high surface area to volume ratio. With regard to joining processes, one characteristic is of particular interest. Nanoparticles show a significantly lower melting and sintering temperature than the corresponding bulk material. Due to this, there is a considerable potential for joining processes at decreased temperatures, especially in comparison to conventional brazing. In the form of suspensions, e.g. pastes, nanoparticles can be applied like braze alloys but achieve a low melting temperatures without the need for melting point depressing elements like boron or silicon, which can lead to the formation of brittle intermetallic phases.

In this work, investigations of nickel nanoparticles are presented, which are intended for a novel type of joining, the so-called nanojoining. Several series of Ni nanopastes are prepared from organic compounds and nanoparticles with mean diameters of 20, 90, 180 and 300 nm, respectively, using ultrasound-enhanced dispersing. With focus on the solvent systems, the feasibility of producing such nanopastes, as well as margins for adjusting their processing properties and results of the thermal behavior are shown. Moreover, first results of joining tests with the Ni nanopastes are presented.

Characterization of Titanium Dioxide for Nanoparticles

Weam Sidahmed Awadalla Sidahmed

University of Khartoum, Sudan

Abstract:

This research aims to study an effect of annealing nanosize titanium dioxide (TiO_2) , Titanium dioxide (TiO_2) is a wide gap oxide semiconductor is an n-type due to oxygen deficiency. It has three phases of the crystal structures including anatase, brookite, and rutile, where the band gap is 3.2 eV for brookite, 3.2 eV for anatase, and 3.0 eV for rutile. The most stable form and the principal source of (TiO_2) are rutile. The metastable anatase and brookite will transform to the thermodynamically stable rutile upon calcination at temperatures exceeding 600°C.

In all three forms, titanium (TiO_4) atoms are coordinated to six oxygen (O_2) atoms, forming (TiO_6) octahedra. Utilize six grams of (TiO_2) material beige color was tope down divided for two parts onewas annealed to 600°C for 4 hours and another let without annealing. The as-prepared samples were further characterized using devices studying (TiO_2) properties, X-Ray Diffraction (XRD), Fourier Transformation Infrared Red (FTIR) and USB Spectrometer. As 0.25 g from both samples was taken and put in (FTIR) to reading transmission and absorption properties, 0.5 g was taken for two samples put in (XRD), and 0.25 g from both samples was taken and used UV-Visible Spectroscopy (USB) to take the readings.

After the properties of the annealed sample were studied and compared to the raw (control powder), this properties were found that the color of the Titanium Dioxide has changed from beige into white as the last one showed fewer impurities and formed Ti-O-Ti vibrational mood which was absent in the control sample. The band gap was recorded and found to be 2.567 eV and 2.568 eV for control and annealed samples respectively.

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Poster Presentations

Solid State Photoreduction of Silver on Mesoporous Silica to Enhance Antifungal Activity

Giulia Quaglia

University of Perugia, Italy

Abstract:

In the present work, an innovative method to prepare Ag^0 nanoparticles as an efficient environmental anti-fouling agent is presented. The synthetic process involves a solid-state Ultraviolet-photoreduction of silver cations to produce Ag^0 nanostructures on a mesoporous silica. In particular, the powder of Ag^+ adsorbed on mesoporous silica, is irradiated at 366 nm, where silica surface defects absorb.

The extinction spectrum of the solid irradiated nanocomposite shows the appearance of a Vis band centered at 470 nm, due to the surface plasmon resonance of Ag⁰ nanostructures; the morphology changes observed in TEM images, associated with the increase of Ag/O ratio in EDX analysis, indicate the photo-induced formation of Ag⁰. The detailed characterization of the materials confirms that the photo-induced reduction of silver cations occurs in the solid state through the activation of silica defects. The nanomaterials are then tested, evaluating their antimicrobial activity using an environmental filamentous fungus, *Aspergillus niger*. The irradiation treatment doubled inhibitory capacity in terms of minimal inhibitory concentration (MIC) and biofilm growth. The antimicrobial properties of silver–silica nanocomposites are also investigated when dispersed in a commercial sealant; the nanocomposites show excellent dispersion in the silicon and improve its anti-fouling capacity for over 60 days.

Modulating Cell Motions Using pH Responsive DNA Origami

Deepak Karna

Kent State University, OH, USA

Abstract:

Cell motions are integral part in proper functioning of different activities in multicellular organisms. Some notable processes include wound healing, immune cell responses, embryonic development and so on. However, certain aberrant cellular migrations are observed during metastatic cancerous conditions in which cells rapidly divide and migrate from place of origin to various other sites. Here, we proposed a unique design to selectively restrict the motion of cancer cells without affecting normal cellular migrations using DNA origamis. To that end, we synthesized a 6-helix bundle of DNA nanospring having a pH responsive behavior. Such characteristic behavior of nanospring was mediated by i-motifs placed in between neighboring piers within origami such that lower pH (nature of cancerous extracellular matrix) lead to formation of its tetraplex structure. Having numerous folded i-motif tetraplexes resulted into coiled nanospring. On the other hand, the normal pH (experienced by extracellular matrix of normal cells) lead to formation of unfolded i-motifs giving rise to a linear nanospring. Next, to direct the motility of cells, we incorporated precisely positioned arginyl-glycyl-aspartic acid (RGD) motifs on the nanospring which could target the integrins, that play significant role in cellular motions. In summary, the coiled nanospring formed during acidic pH resulted into clustering of integrin molecules on cell surface thereby restricting the motion of cancerous cells while the uncoiled nanosprings formed at neutral pH caused declustering of integrins providing no major limitations to the cellular motility. Thus, such a chemo-mechanical modulation exhibited a noble strategy to restrain cancer cell migration follow-up of which assist the on-site therapeutic procedures.

Preparation and Characterization of Stable Nanoliposomal Formulations of Curcumin with High Loading Efficacy: *in vitro* and *in vivo* Anti-tumor Study

Maryam Karimi

University of Maryland, MD, USA

Abstract:

Curcumin (CUR) is a natural hydrophobic polyphenol compound, the main active constituent of turmeric which is isolated from the plant Curcuma longa. CUR has been shown to possess a broad spectrum of biological effects including anti-inflammatory, antioxidant, anti-angiogenic and anticancer properties Despite numerous biological effects of CUR, poor water solubility and bioavailability, short half-life, rapid metabolism and chemical instability are major barriers which limited its clinical applications then liposomes are best Nano carrier. However, the physical and chemical stability of conventional CUR-loaded liposomes for long term storage and their industrial scale-up remain the major obstacle for conventional formulations in these liposomes, CUR was incorporated into the phospholipid bilayer using passive loading methods, which had disadvantages; such as, instability, limited capacity and burst-release profile. Therefore, developing and improved new method for preparation of high loading liposome through solvent-assisted active loading technology (SALT) method, in which drug actively loaded in liposomal core. In this method dimethyl sulfoxide (DMSO) play roles as a drug solvent and membrane permeation enhancer that could effectively enhance the loading of hydrophobic drugs in the internal aqueous of liposome. Liposomal formulations were made using SALT method. Two formulations composed of HSPC: DPPG: Chol: DSPE-mPEG2000 (PG-LipCUR) and HSPC: Chol:DSPE-mPEG2000 (LipCUR) demonstrated good colloidal properties and the CUR-encapsulation of 82% and 89% for PG-LipCUR and LipCUR, respectively. The results showed that both formulations were stable during 6 months storage at 4 °C. The release study showed that the PG-LipCUR and Lip-CUR formulations are relatively stable at pH 7.4. Both formulations had higher cytotoxicity on TUBO and 4T1 cell lines in compassion with normal cells. PG-LipCUR had the higher amounts of CUR cellular uptake than LipCUR. Biodistribution studies showed that both formulations could enhance the half-life of the CUR 2–3 times compared to free CUR. The tumor accumulation of PG-LipCUR was significantly higher than LipCUR. The antitumor activities of liposomes on 4T1 tumor model demonstrated the efficacy of both formulations compared to PBS and free CUR. PG-LipCUR also was more potent in tumor growth delay in comparison with LipCUR. However, combination of the Caelyx® and PG-LipCUR had the most antitumor properties among other treatments. Based on the results, PG-LipCUR could be a promising formulation for the delivery of CUR which also significantly increased the efficacy of Caelyx[®] and merits further investigation.

Quantum Switching in Y-shaped Nanostructures

Trevor McDonough

SUNY University at Buffalo, NY, USA

Abstract:

Using Silvaco Atlas codes with 3D Schrodinger-Poisson electrostatic solver and non-equilibrium Green's function (NEGF) transport simulator, we demonstrated low power switching in a gated Y-shaped one-dimensional ballistic waveguides cut from Al-free InGaAs/InP quantum well (QW). We have evaluated current switching in the devices as a function of modulation doping and temperature. Modulation doping was implemented symmetrically around the QW with 5 nm spacer layers similar to experimentally fabricated test structures. To verify that the solver is correctly treating quantum transport, simulations were executed for different doping levels to control filling of the first few 1D subbands. The resulting conductance we doping plot showed the expected stair-like profile with the height of each step equal to conductance quantum, 7.75×10^{-5} S. We demonstrated the switching of current between branches of the Y-shaped wave guide at gate voltage as low as 10 mV with 1 mV bias applied to the waveguide, and compared these results to estimates based on the overlap of wavefunctions of the stem and the branches. Notably, the most efficient switching occurs when the band and doping profiles have only the first subband discontinuity at the junction results in the first energy level of the branches matching the second partially filled subband of the stem. This results in one order of magnitude ballistic current steering between the degenerate (metallic) semiconductor 1D branches at about 6 mV at low temperature.

Surface Modification and Characterization of Germanium Nanoparticles

Viktoriia Slynchuk

Eberhard Karls University of Tuebingen, Germany

Abstract:

The colloidal germanium nanoparticles are an attractive class of units to create complex materials with unique properties for a variety of applications. A number of different synthetic approaches have been investigated towards achieving Ge-based nanomaterials. Here, we present the functionalization and characterization of colloidal germanium nanoparticles with a small size distribution. The nanoparticles were prepared via disproportionation reaction of metastable subvalent Ge(I)Br solutions. The particles in this way produced can be functionalized, since the surface is terminated by halogen atoms, which can be readily substituted by organic or other functional groups.



Figure: Schematic of the germanium nanoparticles size development ($D = \text{donor} (P^n Bu_3)$).

The surface modification plays an important role in the stabilization of Ge nanoparticles since the overall quality of functional groups is a dominant contributing factor for an applications approach. The substitution reaction with a ligand increases stability of nanoparticles.

A New Reductant in Gold Cluster Chemistry Gives a Superatomic Gold Gallium Cluster

Florian Fetzer

University of Tuebingen, Germany

Abstract:

The desire to design electronic devices decreasing in size demands well characterized building blocks. Metalloid gold clusters have shown great potential due to the atomically precise knowledge of their structure and composition. Studying structure-property relations and synthetic mechanisms of gold clusters requires a variety of structurally resolved compounds.

The gold cluster chemistry is almost completely based on borane-containing reducing agents. To widen the catalogue of metalloid gold clusters, new synthetic procedures need to be designed. We present the first use of the subvalent gallium(I)-compound GaCp (Cp = cyclopentadiene) as reductant in gold chemistry successfully giving the intermetalloid cluster $[Au_9(PPh_3)GaCl_2]^{2+}$. The compound was thoroughly characterized by NMR, single crystal X-ray scattering and mass spectroscopy. DFT calculations support the classification of this compound as an eight-electron superatom cluster.

The easy accessibility of GaCp and the high yield of the resulting cluster renders this system promising for further research towards new metalloid and intermetalloid gold clusters.

Molecular Biology and Microorganisms Brownian Motion Fractal Nature

Bojana Markovic

Serbia and Institute of Technical Sciences of SASA, Serbia

Abstract:

Molecular biology, as a science with research field focused on processes in alive organisms at a molecular level, has a great significance in fundamental and applied research. Nowadays, when the world is facing severe pandemic diseases, molecular biology research and achievements are even more important than ever. Structures and different life functions of microorganisms, like motion, are based on molecular biology processes. There is a great importance to define relation between molecular and microorganisms levels. The idea of our research is to explain the Brownian motion as phenomenon at this level of alive matter. This research is also important for later analysis of Brownian motion at the level of the alive matter and the physical system particles. This is very important from the aspect that the particles in the condensed matter could be treated also as a part of supermicro, nano, molecular structures of microorganisms. As data, we used the experimental results based on some microorganisms motion. Important goal and possible conclusions could be in the direction that we have the phenomenology of Brownian motion which is the effect of structures hierarchy from molecular level through the alive microorganisms structures. From the aspect of the Brownian motion and biomimetic fractals similarities which are existing in nature we can collect important scientific information which basically also integrate the matter particles processes in alive and nonalive systems as well. This will also open the possibility of a new approach in Coronavirus and other potential viruses motion research.

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