Magnetic nanomaterials and their use in advanced composite materials: control of magnetic properties and applications

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ABSTRACT

The use of magnetic nanostructures combined with other materials to obtain composite materials with tailor-made properties has been a very active area of research in recent years. This is because this approach makes it possible to obtain materials with original properties and characteristics that reflect the combination of the properties of the different materials used. In the case of nanostructured magnetic materials, these can be particles, nanowires or three-dimensional structures in which the type of material and its microstructure can be varied in order to modulate their individual magnetic properties. The other material of the composite, which serves as the matrix in which the magnetic material is contained, can be organic or inorganic, hard or soft/flexible and can have multiple shapes, which gives rise to a wide variety of possibilities to fabricate materials with unique properties. In this talk, we will present some examples of these composite materials using nanoparticles or nanowires and discuss different methods of synthesis and fabrication as well as strategies that are used to control and modify their properties and some of their possible applications.

Electron Localization-Delocalization Matrices (LDMs): A Powerful Molecular Descriptor for in silico Design of Materials

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ABSTRACT

An electron localization-delocalization matrix (LDM) is a matrix representation of the complete molecular graph. A complete (molecular) graph links every pair of atoms (vertices) in the molecule - in contrast with the generally-incomplete chemical structure graph which only places a line between atoms considered to be chemically-bonded. The edges (links) of the graph represented by an LDM are electron delocalization channels which exist between every pair of atoms in the molecule (only a subset of these channels coincide with chemical bonds). An LDM, hence, contains information on the electron distribution in the molecule at an atomic/atomic-pair resolution. By feeding the matrix elements of the LDM with electron localization and delocalization indices calculated from numerical Quantum Theory of Atoms in Molecules (QTAIM), the LDM bridges quantum chemistry and chemical graph theory. Due to their sound foundations in physics, LDMs are powerful predictors of molecular and materials properties as diverse as pKa's, boiling points, substituents effects, aromaticity, corrosion inhibitors' activity (including discovery of the active species – Fig. 1), mosquito repellency, UV λmax bathochromic shifts, enzyme catalysis, etc. [1-6]

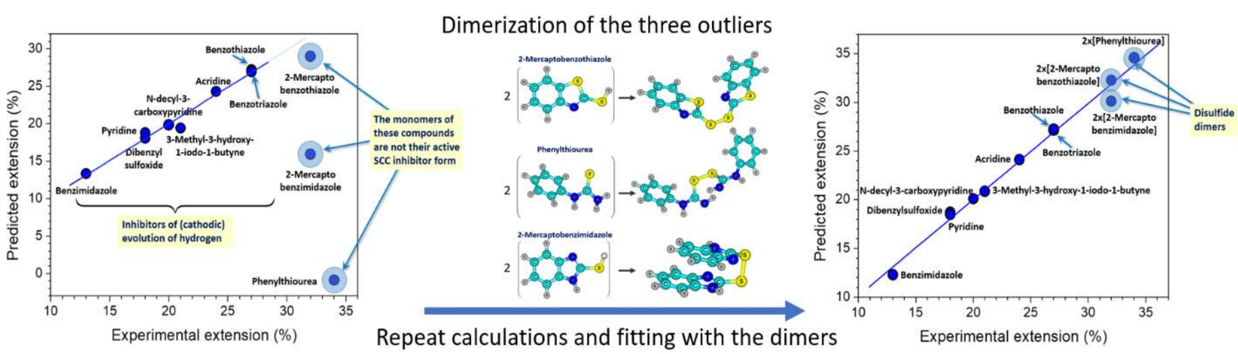

Fig. 1 LDM's PCA eigenvalues regressed against the experimental wire extension before breaking under stress corrosion cracking conditions showing how the inclusion of the correct species "normalizes" the three outliers with -SH groups after their oxidative dimerization at the anode. (Courtesy of Dr. Ronald Cook [1]).

Growth of Wurtzite and Zinc-Blende Phases in III-N Semiconductors by Molecular Beam Epitaxy

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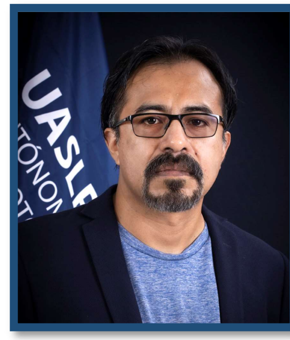
ABSTRACT

In this presentation, we delve into the intricacies of synthesizing III-N semiconductor materials using Molecular Beam Epitaxy (MBE). MBE, renowned for its precision in depositing material at the atomic layer level, is an ideal technique for fabricating heterostructures and nanostructures.

During the first part of our discussion, we present the outcomes of growing wurtzite III-N structures on Si(111) substrates using MBE, with the aid of a radio-frequency (RF) plasma source to generate reactive atomic nitrogen. In the latter segment, we offer insights into the growth of III-N semiconductors on GaAs (100) substrates to induce the formation of the zinc-blende phase. We emphasize the methodology employed to meticulously control the early stages of heteroepitaxy, ensuring a substantial cubic phase content in the resultant GaN. Throughout our presentation, we explore the optical, electrical, and structural properties of nanostructures and heterostructures of III-N semiconductors in both wurtzite and zinc-blende phases. This discussion promises to illuminate the nuances of III-N semiconductor growth via MBE, shedding light on the intricacies of crystal phases and their potential implications for future device technologies.

Exploring Coherent Transverse Coupling in 3D Semiconductor Nanowire Arrays for Quantum Applications



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ABSTRACT

The exploration of quantum coherence in nanostructures is as a critical field with vast implications for the advancement of quantum information, communication, and sensing technologies. Previous studies have predominantly focused on coherent tunneling processes within a limited number of stacked quantum nanostructures such as dots or rings, leading to the formation of delocalized molecular states characterized by robust electron and hole coupling. These interconnected quantum dots and rings, similar to artificial molecules, demonstrate the potential for establishing quantum gates through coherent coupling, thereby laying the groundwork for essential components in quantum technologies. In this talk, we present our latest theoretical findings on nanowire coupling. Our focus is on the coherent transverse coupling in three-dimensional arrays of closely spaced, vertically stacked nanowires. These nanowires are characterized by their discontinuous charge distribution along the axial direction. This particular setup has enabled us to observe a widespread redistribution of carrier populations across various excited states within the nanowire array. Moving beyond theoretical models, we are currently engaged in the development of actual prototypes. This ongoing effort involves utilizing advanced epitaxial growth and nanowire self-assembly methods. While the fabrication of these prototypes is still in progress, it represents a crucial step towards validating our theoretical predictions in practical scenarios. Successfully developing these prototypes will not only enhance our understanding of quantum coherence in nanostructures but will also open new avenues in quantum computing and sensing technologies.

Characteristics of Polymer Microgel-Colloids and Pastes Analyzed through Light Scattering and Superresolution Microscopy

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ABSTRACT

Microgels are among the most studied colloidal and polymeric systems of the past decades [1,2]. Swelling thermosensitive poly(N-isopropylacrylamide) microgels by lowering the temperature provides a unique mechanism for controlling the porosity and size of colloidal particles on the nanoscale. Consequently, these smart microgel particles are being considered for applications ranging from viscosity modifiers and sensing to drug delivery and as models for the glass and the jamming transition of soft colloids.

Here, we present results from light scattering, rheology and in-situ two-color superresolution microscopy of dye-labeled submicron-sized pNiPAM microgels. We use static (SLS) and dynamic light scattering (DLS) to study the swollen microgel's density profile and hydrodynamic size over a large range of temperatures. We show that the q-dependent scattered intensity I(q) can be used to quantitatively model the microgel suspensions' absorbance, unraveling a recently found scaling behavior of the absorbance temperature dependence from UV-VIS spectroscopy data [3]. Moreover, we study the de-swelling of microgels by applying an extra osmotic pressure, suspending the microgels in a high molecular weight dextran solution at different concentrations and we utilize optical tweezers to investigate the interaction potential of microgel particles exhibiting weak interactions [4].

In addition to light scattering, we use direct Stochastic Optical Reconstruction Microscopy (dSTORM) to image single microgels in two and three dimensions, at different stages of the volume phase transition, with a lateral optical resolution of 30nm [2]. Utilizing superresolution fluorescent microscopy enables the examination of individual colloids within a densely packed microgel paste, leveraging the specificity afforded by multi-color dye labelingAs we increase the packing density, we map out the different contributions that allow the dense packing of the soft microgels due to deformation, interpenetration, and compression. Based on a detailed understanding of the local structure and morphology, we can describe the macroscopic elastic properties of dense suspensions over a broad range of densities [5,6].

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Some new insights of informational entropies in chemistry

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ABSTRACT
In this talk, we will focus on the discussion of some of the informational entropies and their possible relationship among some concepts of chemistry such as hardness, chemical potential, among others, which are some of the main ingredients of the chemical reactivity theory. In this regard, we also discuss the use of informational entropies to describe some simple chemical reactions, and how this concept may be linked to important chemical changes, such as the process of bond-breaking and bond-forming.

NANOPLASMONICS: LOCALIZED CONTROL OF LIGHT PROPAGATION AT THE NANOMETER SCALE

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ABSTRACT

The field of nanoplasmonics has undergone significant progress over the past two decades, particularly in the development of nanoplasmonic devices [1]. This evolution has fueled a growing interest in the conceptualization and realization of 2D optics, a captivating notion that aims to retain the operational speeds of classical optics while enabling the seamless integration of elements at the nanometric scale. This dynamic area of research represents a focal point for cutting-edge investigations. In this context, we delve into a comprehensive exploration of individual nanoplasmonic nanostructures, employing a unified approach encompassing numerical modeling, electron beam lithography (EBL) for manufacturing, and meticulous characterization through advanced optical microscopy techniques[2]. While the adherence to a standardized framework may not be a prerequisite for this research, it presents a noteworthy contribution towards establishing unified criteria. This pursuit is instrumental in steering the trajectory of research endeavors towards the holistic development of an integrated nano-optical circuit. By showcasing a segment of this expansive panorama, we present our achievements in nanoplasmonics and the ongoing discourse towards the realization of a unified and integrated nano-optical future. In this talk, we will present nanoplasmonic elements and metasurfaces that have been subjects of our research. Our exploration will encompass a diverse range of topics, including the design and functionality of different nanoplasmonic devices. Additionally, we will touch upon the advancements in metasurface technology and share insights into our investigations in this exciting realm.[Fig.1].

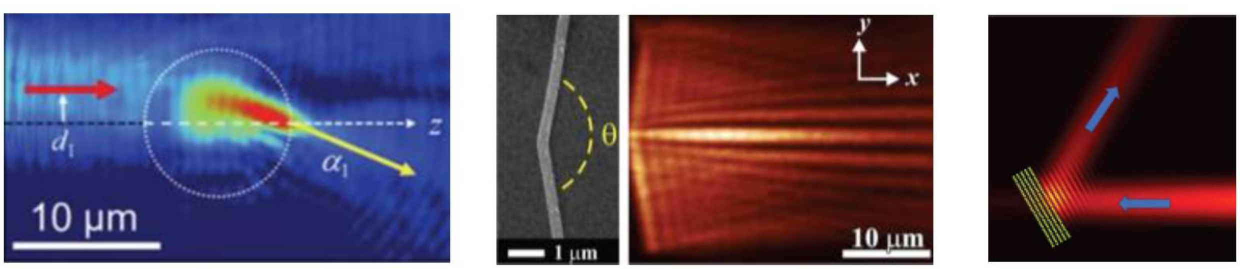

Fig1. Nanoplasmonic devices

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