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C1. Quantum materials: Synthesis to Applications



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C1. Quantum materials: Synthesis to Applications

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SC1-0001 **Invited Talk**

CHARGE TRANSPORT MECHANISMS IN PRINTED THIN FILMS BASED ON TWO-DIMENSIONAL MATERIALS

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Printed electronics has emerged as a pathway for large scale, flexible, and wearable devices promising to unlock a transformational change in the electronics as we know it, and enabling applications in high demand such as wearable electronics[1], Internet-of-Things[2] and smart textiles[3]. Graphene and related two-dimensional (2D) materials offer an ideal platform of novel materials for high performance printed electronics [4,5]. Electronic inks from 2D materials with different electronic properties have been developed to print the different elements of a device: semiconducting or semimetallic inks in the active layer, insulating inks for dielectrics, and conducting inks for electrodes. However, the complexity of the ink formulations, the three-dimensional assembly of the 2D flakes and the polycrystalline nature of the resulting thin films, have made it difficult to examine charge transport in such devices so far [6], therefore impeding an accurate and controllable design of electronic devices.

In this talk I will describe the charge transport mechanisms of surfactant- and solvent-free inkjet-printed thin-film devices of representative few-layer graphene (semi-metal), molybdenum disulphide (MoS_2 , semiconductor) and titanium carbide MXene (Ti_3C_2 , metal) by investigating the temperature, gate and magnetic field dependencies of their electrical conductivity.[7]

Charge transport in printed few-layer MXene and MoS_2 devices is dominated by the intrinsic transport mechanism of the constituent flakes: MXene exhibits a weakly-localized 2D metallic behaviour at any temperature, whereas MoS_2 behaves as an insulator with a crossover from 3D-Mott variable-range hopping to nearest-neighbour hopping around 200 K. On the other hand, charge transport in printed few-layer graphene devices is dominated by the transport mechanism between different flakes, which exhibit 3D-Mott variable range hopping conduction at any temperature.[7] These results establish the fundamental mechanisms responsible for charge transport in inkjet-printed devices made of 2D material, enabling the controlled design and engineering of future printed electronics based on 2D materials, and paving the way to new types of flexible electronic devices.

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Keywords: 2D materials, Transport, Printed electronics

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SC1-0002

CHARGE AND MAGNETOTRANSPORT IN HYBRID VAN DER WAALS HETEROSTRUCTURES

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The rise of graphene and related 2D materials makes it possible to form heterostructures held together by weak interplanar van der Waals (vdW) interactions. The interactions of such 2D layers with adventitious contaminants is able to exert a strong effect on its major electronic characteristics [1]. However, the controlled incorporation of ordered organic molecules within these systems holds an immense potential. Whilst nature offers a finite number of 2D materials, an almost unlimited variety of molecules can be designed and synthesized with predictable functionalities [2-3]. The possibilities offered by systems in which continuous molecular layers are interfaced with inorganic 2D materials to form hybrid organic/inorganic van der Waals heterostructures are emphasized. Similar to their inorganic counterpart, the hybrid structures have been exploited to put forward novel device architectures. Moreover, specific molecular groups can be employed to modify intrinsic properties and confer new capabilities to 2D materials. I will give a brief overview of how molecular self-assembly at the surface of 2D materials can be mastered to achieve precise control over position and density of (molecular) functional groups, paving the way for a new class of hybrid functional. In particular, within such vdW heterostructures, currently assembled by mechanical superposition of different layers, periodic potentials naturally occur at the interface between the 2D materials. These potentials significantly modify the electronic structure of the individual 2D components within the stack and their alignment, thus offering the possibility to build up hybrid and novel materials with unique properties. Furthermore, I will also show how dynamic light-switchable supramolecular lattices can be created on graphene thus imparting novel functionalities to the pristine material.

References

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Keywords: quantum materials, devices, van der Waals heterostructure

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SC1-0004 **Invited Talk**

SUPERCONDUCTIVITY AT CARRIER DENSITY 10^{17} cm^{-3} IN QUASI-ONE-DIMENSIONAL $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$

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Superconductivity at very low carrier density is a rare and fascinating phenomenon that is of considerable importance and interest in condensed matter physics. The conditions of high density of states and effective screening of Coulomb repulsion, both key ingredients of stable Cooper pairing in the BCS theory, may not be met at low carrier density. Thus, such systems may also harbor unconventional electron pairing (e.g. non-phononic) or pairing without phase coherence as a precursor to Bose-Einstein condensation. An intriguing route toward extreme low-density (and possibly unconventional) superconductivity may be found in quasi-one-dimensional metals for which density-wave instabilities compete for the ground state and can lead to gapping of substantial portions of the Fermi surface (FS), leaving a residual (reconstructed) FS comprising a very small carrier density. Our work¹ highlights a novel material in this unusual category: $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$ ($T_c=2 \text{ K}$) (also known as "lithium purple bronze" or "LiPB"). We present both electrical and thermoelectric magnetotransport measurements that reveal superconductivity to occur at carrier density $2 \times 10^{17} \text{ cm}^{-3}$, among the lowest known for any superconductor, and four orders of magnitude lower than is expected from its chemical valence and band structure.² With its exceptionally large ratio of superconducting to Fermi temperature, $T_c/T_F \approx 0.1$, LiPB is properly placed at the top of a very small group of superconductors (including cuprates, heavy-fermion and Fe-based superconductors) for which this ratio falls in the BCS-BEC crossover regime and for which pairing is believed to be spin mediated.

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Keywords: superconductivity, low dimensionality, transport phenomena

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SC1-0005

FLAT-BANDS IN DECAGONAL QUASICRYSTALS

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The emergence of superconductivity in twisted systems opens new ways and possibilities to study this phenomenon. Since the discovery of high T_c superconductors, it was acknowledged that the multiple layer structure of the system plays a fundamental role in the emergence of the superconducting state. The recent discovery of superconductivity on twisted bilayer graphene, adds a twist to the multiple layer systems, giving rise to the appearance of flat bands, which is responsible for the rising of correlated states. Superconductivity was also discovered on Quasicrystals (QCs), which are systems that show no periodicity, neither they're amorphous. Almost 40 years has passed since the discovery of quasicrystals. Their structure was characterized, the stability has been studied, and the superconducting states have been found. The finding of naturally occurring quasicrystals has been added to the list. The decagonal quasicrystals are a type of QCs that are periodic in one direction and quasiperiodic in two directions. The Penrose tessellation is the two dimensional most used model to study QCs due to presenting the same diffraction pattern as QCs. In this work, we model the coupling of two Penrose lattices, and twist one respect to the other until a Moiré pattern appears. We calculated the spectrum and eigenvectors of the system and analyse the electronic states of interest. The density of states is also studied.

Keywords: flat-bands, quasicrystals, superconductivity

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SC1-0006 **Invited Talk**

EFFECT OF SUPERCONDUCTIVITY ON MAGNETISM IN A SUPERCONDUCTING/MAGNETIC HYBRID

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The capacity to control magnetism via superconductivity is a highly sought effect. Introducing Cooper pairs with antiparallel spins into a ferromagnet generally leads to a parallel realignment of spins, resulting in subtle changes to the ferromagnetic order close to the interface. This study tackles a longstanding, intricate issue: the manipulation of magnetic order through superconductivity. We achieve this by leveraging competing interactions in trilayer thin films composed of LPCMO/YBCO/LPCMO, where LPCMO stands for $\text{Pr}_{0.5}\text{La}_{0.2}\text{Ca}_{0.3}\text{MnO}_3$ and YBCO represents $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$. We discover that in the coexistence phase of LPCMO, characterized by the presence of both ferromagnetic-metallic and antiferromagnetic-insulating domains, proximity to a superconducting YBCO film significantly reduces the coercivity field of LPCMO's ferromagnetic phase. This phenomenon is attributed to increased metallicity in LPCMO, which leads to larger magnetic domains and thus, a reduction in magnetic anisotropy within the LPCMO layers. These findings illustrate that magnetic anisotropy in a ferromagnet can be modulated by its proximity to a superconductor when the energy levels are comparable.

Keywords: superconductivity, magnetism, hybrid

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SC1-0008 FERROMAGNETIC AND HALFMETALLIC CHARACTER AT AIP/CrP(001) INTERFACE

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The structural, electronic, and magnetic properties of the epitaxial growth of zinc-blende CrP onto the AIP (001) surface are investigated by first-principles spin-polarized calculations. When two layers of CrP were deposited in the ZB phase, the system became ferromagnetic (FM). Also, it was found that the (rocksalt) RS configuration is unstable due to the large lattice mismatch. The thermodynamic stability of the early stages of the growth and interface formation were investigated using the Surface (SFE) and Interface Formation Energy (IFE) Formalism. Our results found that the epitaxial growth is feasible at Al-rich and Cr-poor conditions. The magnetic and electronic analysis of the stable interface found a ferromagnetic interface with half-metal characteristics with a large band gap of ~ 1 eV for the minority spin; these characteristics could induce a 100% spin-polarized current around the Fermi level. Also, the estimated Curie temperature is larger than 2700 K. Thus, this interface is ferromagnetic with polarized spins aligned in the in-plane direction via a d-p-d exchange coupling mechanism. Most interestingly, interface also exhibits halfmetallicity with pseudo anisotropic topological Dirac cones residing in the spin majority channel. Our findings demonstrate that the CrP/AIP is a suitable candidate to be implemented in different spintronic devices that operate at room temperature or higher.

Keywords: ferromagnetic, halfmetallicity, topological

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SC1-0009 FIRST PRINCIPLES STUDY OF THE ELECTRONIC AND MAGNETIC PROPERTIES OF TRIPLY-LINKED IRON PORPHYRIN TAPES

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Porphyrins are macrocyclic and aromatic molecules of significant importance in different biological and chemical processes. Interestingly, metalloporphyrins can be used as building blocks units due to their unique versatility, allowing the formation of a variety of nanostructures with different dimensionalities. These nanostructures have shown optimal characteristics for their use as components in molecular electronic devices. In particular, the one-dimensional triply-linked porphyrin tapes, present a small experimental value of the energy gap; such characteristic translates into a high conductivity. In this work, we study the electronic and magnetic properties of triply-linked iron porphyrin tapes. The periodically aligned Fe atoms and the small value

of the magnetic exchange coupling constant preludes the behavior of a Quantum Spin Liquid (QSL). Thus, computational simulations based on Density Functional Theory (DFT) were performed, using the method of pseudopotentials and plane waves as implemented in the Quantum ESPRESSO code. The General Gradient Approximation (GGA) was used as the exchange correlation functional with the application of the Hubbard correction U for the Fe 3d states. The Hubbard parameter was self-consistently computed via the Density Functional Perturbation Theory (DFPT) method.

Keywords: Nanostructures, Magnetism, Quantum Spin Liquid

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SC1-0010

MODEL BASED ON DIFFERENTIAL EQUATIONS TO EXPLAIN THE QUENCHING OF LUMINESCENT POROUS SILICON IN AN ETHANOL-WATER SYSTEM

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Luminescence quenching in porous silicon has been widely employed due to its sensitivity to numerous molecular species acting as quenchers. Various molecular interactions can induce luminescence quenching, including excited state reactions, molecular rearrangement, energy transfer, complex formation in the basal state, and collisional quenching. Collisional inhibition, also known as dynamic process, occurs when the excited-state silicon is deactivated upon contact with another molecule in solution, called quencher. To explain the interaction of luminescent porous silicon with quenchers in an ethanol-water system, a model based on differential equations was proposed, which is a conventional tool for exploring luminescent processes. This method focuses on analyzing the population density of each energy level involved.

Photoluminescence inhibition tests were conducted using ethanol and water. The amount of water was kept constant at 10, 11, and 12 mL, while the amount of ethanol in each batch varied. Spectra were acquired using a fluorescence spectrometer (Varian-Agilent Cary Eclipse) with an excitation wavelength of 360 nm, employing a mount designed for liquids at room temperature. The collected measurements were analyzed and fitted to the proposed model. The findings indicate a strong alignment between the proposed model and the collected data.

Keywords: porous, Silicon, quenching

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SC1-0011 **Invited Talk**

QUANTUM MATERIALS IN MEDICINE: HUMAN RESULTS

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Quantum materials have been widely researched for magnetic, topological insulators, semiconductors, energy, and other applications. However, they are rarely (if at all) used to describe improvements to medicine. This invited talk will discuss the numerous applications and promises of quantum materials in medicine. Specifically, it will discuss how quantum materials are being used at topological insulators in sensors to detect infection, inflammation, or tissue growth. In such applications, electron distribution can be controlled through quantum mechanics via external stimuli to alter electron orbitals and electronic properties. Quantum materials are also being used as self-power for such implantable sensors. Further, this talk will highlight research in which magnetic quantum dots have helped prevent, diagnose, and treat numerous diseases. It will also introduce new mathematical formulas in which protein adsorption to quantum materials which control cell functions (such as cancer cell death) can not be described through conventional models. The unique surface energy generated by quantum materials will be demonstrated and how such unique surface energy can control cell functions throughout the body to treat diseases will be emphasized. Human data will be emphasized in this presentation due to its high impact. In summary, this talk will discuss what has already been accomplished in medicine by quantum materials and where the promises lie for the future.

Keywords: medicine, human, quantum

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SC1-0012

SYNTHESIS OF QUANTUM DOTS BY PULSED LASER ABLATION IN LIQUIDS

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To create and develop new quantum materials with well-defined crystalline structure and physico-chemical properties that cannot be achieved by using traditional wet-chemistry techniques, pulsed laser ablation is going to be used. The focus of this talk will be on the synthesis of bismuth telluride quantum dots by pulsed laser ablation in liquids. The quantum confinement has been confirmed by Raman spectroscopy. The size of the quantum dots has been determined by transmission electron microscopy.

Keywords: quantum dot, laser, bismuth telluride

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SC1-0014 **Invited Talk**

CHIRALITY TRANSPORT AT THE NANOSCALE

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Chirality is a geometric property of matter that can be present at different scales, especially at the nanoscale. Here, we investigate the manifestation of chirality in electronic transport through a molecular junction.

Spinless electronic transport through a chiral molecular junction is not enantiospecific. However, when a chiral metal cluster, C₃-Au₃₄, is attached to the source electrode, a different response is obtained in spinless electronic transport between R and L systems: this indicates the crucial role of chiral clusters in triggering enantiospecific spinless electronic transport. Using the non-equilibrium green's function method, theoretically we characterized this phenomenon by calculating the transmission and conductance of spin-unpolarized electrons.

Keywords: Chirality, Electronic transport, First principle-based calculations

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SC1-0015 **Invited Talk**

SINGLE-WALLED CARBON NANOTUBE HYBRIDS VIA ENCAPSULATION: ON THEIR OPTICAL AND ELECTRONIC PROPERTIES

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The advances on the science and application of carbon nanotubes within the last three decades have brought to reality the production of materials approaching the theoretical predictions. Single-walled carbon nanotubes (SWCNTs), in particular, have outstanding electronic and optical properties. For instance, enhancing the photoluminescence of SWCNTs can bring to reality more than one ground breaking application in fields like biology and optoelectronics. However, the optical properties of these materials are strongly related to their morphology and intrinsically to their diameter. A potential way to gain control of properties like PL is the encapsulation of molecules or nanostructures in the tube's hollow core but there are very small diameter tubes where this is not straightforward. We will discuss how new hybrids composed by SWCNTs and confined structures like nanowires, graphene nanoribbons or linear carbon chains have been developed. We will discuss on the optical response of these materials and I will describe how phenomena like a diameter-dependent enhancement of the PL can be induced by energy transfer.

Keywords: single-walled carbon nanotubes, spectroscopy, charge transfer

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SC1-0016 **Invited Talk**

CARBON QUANTUM DOTS FOR SENSING POLLUTANTS IN THE AQUEOUS ENVIRONMENT

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Rapid industrialization and untreated industrial effluents loaded with toxic and carcinogenic contaminants, especially pesticides, heavy metals, and dyes that discharge into environmental waters, have led to a rise in water pollution, substantially impacting marine life and humankind. Photophysical properties are one of the most successful methods that help to detect such contaminants. In recent years, semiconductor quantum dots have been substituted by carbon dots (CDs) as optical sensors due to the ease of formation, cost-effectiveness, possible sustainability and scalability, much lower toxicity, and, above all, its high capacity to harvest light through electron transfer that enhances the lifetime of the photogenerated charge carriers. A better understanding of the properties of the CDs and their role in the optical sensing of contaminants is required to form controllable structures and adjustable outcomes. The focus of this talk is on CDs obtained from different sustainable green as well as chemical precursors. Besides the present research development in the field, potential challenges and future perspectives will also be discussed.

Keywords: Carbon Quantum Dots, Environmental Sensor, Optical Sensor

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SC1-0017 SEDIMENTATION, DETECTION AND REDUCTION OF WATER CONTAMINANTS WITH PITHECELLOBIUM DULCE CARBON DOTS

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Pollution by metal ions and organic pollutants is a continuous growing problem, and one possible way to counteract it, is the development of new environmentally friendly and low-cost techniques, which are required for the detection and also for the drop of the levels of these pollutants in water. Carbon dots (CDs) have photoluminescence (PL) and other properties that make them able and suitable for use as optical nano sensors, reducing agents or even as promoters for the precipitation of metal ions (M^+) for potential removal from water. The development of CDs derived from Pithecellobium Dulce (PD) leaves and its applications is presented. These CDs were used in the direct detection of Cr^{6+} and 4-NP, as well as the identification of Fe^{3+} by complete quenching, Sn^{2+} identification is by decreasing the PL and by redshift of the signal, conversely the Zn^{2+} signal increases and present a displacement to the blue color. With ON-OFF-ON arrangement, the PL can be recovered by Zn and paraquat (pesticide), making possible to identify its presence of this pollutants. The CDs were also used in the precipitation of Fe^{3+} , Pb^{+2} , and Sn^{+2} , therefore there is a possibility to remove this M^+ . The X-ray photoelectron spectroscopy (XPS) characterization suggest there is a reduction of Fe^{3+} to Fe^{2+} and the Pb^{+2} to Pb^0

Keywords: Adsorption, Heavy metals, Carbon dots

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SC1-0018 ACETONE FLUORESCENT SENSING WITH CARBON-DOTS-AUNPS HYBRID COMPOSITE

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Acetone is a ketone body that has recently attracted attention as a potential non-invasive Diabetes biomarker; thus, novel nanomaterials for sensitive acetone detection are attractive for medical purposes. Carbon Dots (CDs) are carbon nanoparticles with less than 10 nm exhibiting remarkable properties such as high quantum efficiency, and fluorescence. Since CDs have showed spectral and surface recognition towards acetone, in this work, we proposed a hybrid nanocomposite of CDs doped with nitrogen, functionalized with AuNPs as sensitive and selective acetone fluorescent sensor. CDs were obtained by hydrothermal method using rGO as precursor. AuNPs were synthesized by the Turkevich Method. The CDs-AuNPs were characterized by HRTEM, XRD, FT-IR, Raman spectroscopy and UV-Vis. The average size for CDs and AuNPs was 16 nm and 16.5 nm respectively. The Raman spectra of CDs showed a characteristic D and G band at 1337 cm⁻¹ and 1593 cm⁻¹ respectively. FT-IR spectra of CDs show absorption peaks of the groups C=O at 1716 cm⁻¹, C-O at 1308 cm⁻¹, C-O-C at 1045 cm⁻¹ and O-H at 3300 cm⁻¹. The optical properties of the materials showed a well-defined plasmon band for AuNPs at 560 nm, and 236 nm for CDs; meanwhile, the CDs-AuNPs showed an absorption band at 528 nm. CDs exhibited an excitation wavelength-dependent luminescent behavior with a maximum emission of 624 nm obtained towards an excitation wavelength of 532 nm. The performance of CDs-AuNPs was tested with fluorescence spectroscopy by adding 1, 5 and 10 ppm of acetone. The addition of 400 ppm of acetone slightly quenched the fluorescence intensity of CDs; therefore, we assume that a FRET process take place in the CD-Acetone system. The CDs-AuNPs showed a detection and a quantification limits of 0.306 ppm and 0.308 ppm respectively, making it a promising material for sensing acetone at low concentration.

Keywords: Nitrogen-doped Carbon Dots, Nanohybrids, Fluorescence

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SC1-P005

OPTICAL DETECTION OF ACETONE, ETHANOL AND METHANOL USING CARBON DOTS OF EICHHORNIA CRASSIPES

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At the present time the Carbon dots' (CDs) applications are highly interesting because their composition natural sources could be used as precursors obtaining CDs with excellent properties (low oxicity, biocompatibility, high solubility in water). The used method of production is friendly with the environmental, due to one step carbonization of green resources (biomass) as precursors. The aquatic Lily (Eichhornia crassipes) is known for absorbing the O₂ and N₂ that is present in the water bodies. This plant grows in polluted waters and adapts it to various environments.

Despite being considered a weed due to its excessive growing. This plant is used in processes to obtain

biogas, biofertilizer, bioplastics, in this case CDs. CDs due to their starch, cellulose and protein content, they server as a water-soluble and highly flourescent precursor, allowing to be applied as an excellent sensor.

As contaminants, organic solvents are chemical products that are harmful to humans, as they are present in water bodies, drinks, blood, pharmaceutical products, among others; They can cause serious secondary reactions even death, so their detection is important.

In this work, the green synthesis was carried out using Eichhornia crassipes as a precursor. The CDs were used to analyze acetone, ethanol and methanol by its optical properties as. This sensor was able to detect of 0.05% acetone, 1% ethanol and 0.5% methanol.

Keywords: Green, Detect, CDs

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SC1-P006

GREEN CARBON QUANTUM DOTS (CQDs) SYNTHESIS FROM BEETROOT CARBONIZATION AND THEIR APPLICATION AS METAL ION SENSING (Cu²⁺)

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The present investigation shows a novel synthesis method for the production of carbon quantum dots (CQDs) from beetroot waste (bagasse), offering an economical and environmentally friendly alternative. This process involves a low-cost synthesis-functionalization using different carbonization times and temperatures, resulting in water-dispersible CQDs with fluorescence properties. The obtained CQDs exhibit an interesting range of emissions in colors such as violet and blue, when they are excited at 325 nm.

The nanoparticles were characterized by UV-Vis and PL spectroscopy to determine their absorption and emission wavelengths, respectively. Additionally, to determine their composition, FT-IR spectroscopy measurements were conducted, identifying the carbonyl groups of the betalainic functional groups present in the beetroot as responsible for the photoluminescent properties of the CQDs. It was also determined by Raman spectroscopy that these nanomaterials are primarily composed of graphitic carbon and oxygen functional groups. Finally, HR-TEM images of one of the samples were obtained to determine their morphology and particle size.

In addition to their innovative synthesis, the CQDs were evaluated for their potential application as metal ions sensing, particularly Cu²⁺. The decrease in luminescence emission intensity in the presence of these metal ions suggests their viability as sensing devices. This research not only offers a promising solution for water treatment using biomass waste, especially relevant in developing countries where polluted water is increasingly abundant, but also suggests new possibilities in the field of metal ion sensing. Overall, the results highlight the versatility and potential of beetroot waste-derived CQDs, opening the door for future research to further explore their applications in many scientific and technological fields.

Keywords: Carbon quantum dots (CQDs), Beetroot, Oxygen functional groups

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SC1-P007

FINE-TUNING BAND GAP: EXPLORING THE INFLUENCE OF SYNTHESIS CONDITIONS ON BIMETALLIC QUANTUM DOT DEPOSITION ON TiO₂-BASED NANOSTRUCTURES

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Quantum dots display distinctive optical properties stemming from confinement effects, manifesting as the emission of light across a spectrum of colors, efficient absorption of visible light, and enhanced electron excitation. Consequently, they find widespread application in high-fidelity display screens, high-output LED lighting, next-generation solar cells boasting heightened efficiency, contrast agents in biomedical imaging methodologies, and sophisticated sensors and detectors renowned for their high sensitivity and selectivity. In our study, we employed wet routes (specifically sol-gel and hydrothermal methods) to synthesize silver and iron quantum dots, which were subsequently dispersed onto TiO₂-based nanoparticles. We investigated the impact of synthesis temperature on the size of the metal particles and examined how this factor influences optical properties, including the width of the bandgap. X-ray diffraction (XRD) analysis revealed the presence of potassium titanate (K₂Ti₈O₁₇ and K₂Ti₆O₁₃) nanorods. Field emission scanning electron microscopy (FESEM) demonstrated a size distribution smaller than 10 nm, while elemental mapping highlighted variations in the distribution of Ag and Fe particles. High-resolution transmission electron microscopy (HRTEM) images showcased the uniform dispersion of metal particles on the potassium titanate nanorods, allowing for precise size determination, averaging less than 2 nm. Characterization of optical properties via UV-Vis spectroscopy indicated a reduction in the bandgap energy in the range of 3.6-1.88 eV. This decrease was ascribed to the shift of the conduction band towards lower energies and the introduction of intermediate energy states within the bandgap. The impact of synthesis temperature revealed that materials produced at lower temperatures exhibited the smallest band gap values. Similarly, bimetallic particles yielded lower band gap values compared to individual metal particles. These findings are pivotal for the fabrication of silver and iron quantum dots dispersed on potassium titanate nanorods, thereby enhancing visible light absorption and lowering the bandgap energy.

Keywords: Bimetallic quantum dots, TiO₂-based nanostructures, Reduced band gap energy

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SC1-P009

GREEN SYNTHESIS OF GRAPHENE OXIDE QUANTUM DOTS AND ITS INTERACTION WITH ACETYLSALICYLIC ACID

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Graphene oxide quantum dots (GOQDs) were obtained by exfoliating carbon obtained from farming industry waste such as orange peel, coffee grounds and wheat husk. The conjugation between the GOQDs and acetylsalicylic acid was carried out with heat treatment at 100 °C with magnetic stirring for 3 hours. The X-ray diffraction analysis presented two peaks at 23 and 43° related to graphite oxide, the Raman spectrum presented two bands D (1320 cm⁻¹) and G (1580 cm⁻¹) also associated with graphite oxide, after carbon exfoliation, two bands were found in the UV-Vis spectrum at 267 and 330 nm corresponding to transitions of the π - π^* and n - π^* type generated by the C=C, C=O and C=N groups associated with GOQDs. On the other hand, transition energies between 2.19 and 2.83 eV were found using fluorescence spectroscopy. After the conjugation of the GOQDs and acetylsalicylic acid, FTIR spectroscopy showed significant changes in the bands between 1630 and 1660 cm⁻¹ associated with amide I and vibrations of the C=N, C=N, C=C, C=O bonds, C-N and C=O; as well as at 1027 cm⁻¹ due to C-H bonds, in the conjugate changes were observed at 1755 cm⁻¹ associated with C=O vibrations of the acetyl and carboxyl functional group of acetylsalicylic acid, which indicates that the active functional groups are maintained for achieve anti-inflammatory activity. By UV-visible spectroscopy, absorption bands were identified at 202, 229 and 295 nm associated with the bonds of the carboxyl and ester functional groups, as well as the aromatic ring of acetylsalicylic acid. In the conjugate, changes were observed in the 295 nm bands associated with to the aromatic ring of acetylsalicylic acid and in the 229 nm band associated with the carboxylic acid, as well as to the fluorescence centers of the coupling between acetylsalicylic acid and the GOQDs. This makes GOQDs strong candidates as drug nanocarriers or specific biomarkers due to their high fluorescence.

Keywords: GOQDs, acetylsalicylic acid, biomarkers

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SC1-P011

STRUCTURAL ANALYSIS OF YBCO SUPERCONDUCTING NANOPARTICLES

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YBaCuO superconducting nanoparticles and thin films were synthesized by mechanical grinding and sputtering respectively from an initial volumetric sample synthesized by solid state reaction, in a "top-down" synthesis process, which were oxygenated at a temperature of 950°C. Morphological analysis were made by scanning electron microscopy, to know the structural changes of the particles as a function of grinding time, nanoparticles with sizes between 384-827nm were obtained. Additionally, UV-vis spectroscopy and Xray diffraction analysis were carried out. Magnetic measurements showed a reentrant superconducting effect in both ZFC and FC measurement modes, below 10K in the smallest nanoparticles

Keywords: Nanoparticles, Thin films, superconductivity

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SC1-P012

EXPLORING GRAPHENE QUANTUM DOTS-IONIC LIQUID HYBRID NANOMATERIAL FOR ENHANCED ANION DETECTION IN WATER

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Ensuring the quality of water resources is of paramount importance for public health and environmental sustainability. Graphene quantum dots (GQDs) have emerged as promising nanomaterials for sensing applications due to their unique optical and electronic properties, particularly for heavy metals detection in water. In this study, we explore the development of nitrogen GQDs (N-GQDs)-Ionic Liquid (IL) hybrid nanomaterials for enhanced detection of anions in water. The hybridization of GQDs with ILs offers synergistic advantages, combining the excellent optical properties of GQDs with the tunable chemical functionalities of ILs. Observing enhancements in fluorescence intensity and selectivity.

Our approach involves the synthesis and characterization of NGQD-IL hybrids using a facile and scalable one-pot hydrothermal method. Then, the nanomaterials are evaluated for fluorescence quenching in water in the presence of sulfur anions, currently assessing only the decrease in fluorescence intensity, demonstrating their potential for environmental sensing applications for anion detection.

Preliminary results show promising enhancements in the fluorescence of N-GQD@IL compared to N-GQD, characterized by UV-Vis, FT-IR, PL, and Raman spectroscopy, and fluorescence quenching in water with sulfur presence detected by PL spectroscopy, demonstrating their structural presence and behavior toward anions. The proposed nanomaterials offer a novel approach to address the challenges of anion detection in water, particularly in the context of shallow well water monitoring. Overall, our study provides valuable insights into the advances in novel GQDs-IL nanomaterials and the development of advanced nanomaterial-based sensors for environmental monitoring applications.

Keywords: Graphene quantum dots, Anion detection, Ionic Liquid

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SC1-P013

GREEN SYNTHESIS AND STUDY OF LUMINESCENT PROPERTIES OF GRAPHENE QUANTUM DOTS

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Quantum dots (QDs) have a high light conversion coefficient and their reemitted light tends to have a very

narrow spectrum. The electronic characteristics of graphene are associated with the linear dispersion of charge carriers. To date, the graphene is considered one of the main candidates for its application as an element of nanoelectronics of the future. The interest in these structures is mainly due to their small size and intriguing electronic, luminescent and mechanical properties. Pure graphene is of interest as a very efficient sensor, while graphene quantum dots (GQDs) with a modified surface can be used in semiconductor electronics as a basis for organic diodes, light emitters, transistors, for atomic force microscopes, biosensors and chemical sensors. GQDs are important probe particles for imaging biological objects and applications such as biosensors. Their advantages are high luminosity, good biocompatibility, and low toxicity. Nowadays, the current mechanism of luminosity of objects containing nanostructured carbon remains open and debatable. The production methods of graphene quantum dots involve the use of toxic compounds, such as acids (HNO_3 , H_2SO_4), KMnO_4 , sodium borohydride, hydrazine hydrate and dimethylhydrazine. The use of methods based on these substances is associated with risks to the environment and human health. The objective of this research was the “green” method synthesis of GQDs with luminescence properties. During the experiment, ultrasound was applied for 0.3-12 hours to the materials: carbon black or graphite with or without reducing agents {teraphthal (soluble cobalt phthalocyanine containing -COONa groups) or ascorbic acid} and microwave irradiation (2.45 GHz) for 20-60 min. The obtained nanoparticles (5-7 nm in size) with blue luminescence were characterized by FTIR spectroscopy, UV-vis spectroscopy, Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). The presence of nitrogen in the GQDs (N-GQDs) was analyzed and detected, showing dependence on theraphthal concentration.

Keywords: Graphene quantum dots, Theraphthal, Luminescence

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SC1-P014

GREEN SYNTHESIS OF CARBON QUANTUM DOTS FROM MULTIWALLED CARBON NANOTUBES FOR PHOTOTHERMAL CANCER THERAPY AND IMAGING

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This study introduces a novel approach to synthesize carbon quantum dots (CQDs) via a green synthesis method utilizing multiwall carbon nanotubes (MWCNTs) as the precursor material. The synthesis process involves the combination of teraphthal, ascorbic acid, and distilled water in a 1:1:1 ratio, followed by ultrasonication for varying durations (3, 6, 9, and 12 hours). Characterization through Fourier-transform infrared (FTIR) analysis and UV-visible spectroscopy revealed a significant blue shift in the transmittance spectra, indicative of reduced particle size. While the synthesized CQDs displayed remarkable photoluminescence properties, our investigation extends to exploring their potential applications in photothermal cancer therapy and imaging. CQDs can efficiently convert absorbed light into localized heat, offering promising opportunities for precise tumor targeting in photothermal therapy while minimizing damage to surrounding healthy tissues. Additionally, their inherent imaging capabilities hold great potential for real-time visualization of the tumor microenvironment, facilitating early detection and monitoring of therapeutic responses. The adoption of the green synthesis method in this study not only ensures environmental sustainability but also offers scalability and cost-effectiveness. Furthermore, the utilization of MWCNTs as the precursor material introduces an innovative aspect to the synthesis process, potentially enhancing the

functionality and properties of the resulting CQDs.

This research represents a significant advancement in nanomedicine, providing a sustainable and efficient method for producing CQDs with enhanced properties. By extending the application scope to include cancer therapy and imaging, we aim to contribute to the development of novel and effective nanomaterial-based approaches for cancer diagnosis and treatment. Future studies will focus on experimental validation and optimization of these applications, paving the way for improved cancer therapeutics and imaging technologies.

Keywords: Carbon quantum dots, Multiwall carbon nanotubes, Photothermal therapy

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SC1-P015

LIGAND INDUCED CHIRAL QUANTUM DOTS: USING ENVIRONMENTAL FACTORS TO TUNE CHIROPTICAL PROPERTIES

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Chiral semiconducting quantum dots (QDs) coated with various ligands have become key materials in various applications such as biosensing and biorecognition, imaging, asymmetric catalysis, optoelectronic devices, and spintronics. The surface modification with small organic molecules plays an intermediary role in tuning the electronic, optical and chiroptical properties of the QDs. To engage the full potential of the unique properties of chiral nanomaterials and enable their preparation with desired chiroptical characteristics, it is essential to understand how to control the transfer of chirality from chiral molecular ligands at the surface of nanocrystals to the electronic states of QDs. We will present our recent studies on the significance of both solvents and counterions in transferring chirality from chiral molecular ligands to achiral semiconductor QDs. We demonstrate tuning chiroptical, optical and physical properties of dual ligand-coated quantum dots with variable solubility, ranging from hexane to water. This work can lead to the diversified use of ligand-induced chiral quantum dots in various fields.

Keywords: chiral quantum dots, circular dichroism, ligand exchange

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SC1-P017

NANOGRAPHITE: A STUDY OF ITS OPTICAL PROPERTIES THROUGH PHOTOLUMINESCENCE SPECTROSCOPY

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It is presented a comprehensive analysis through photoluminescence spectroscopy in nanographite (NG). This approach not only involves optical characterization but also the understanding of the various mechanisms underlying this material of nanostructure, which is relevant for its application in multiple fields.

The exploration of the optical properties of nanographite was carried out using photoluminescence spectroscopy, employing different excitation wavelengths that allowed obtaining various emission spectra. A full width at half maximum (FWHM) of approximately 40 nanometers was observed, accompanied by a shift towards the infrared and a decrease in its intensity. This FWHM can be attributed to the various carbon-carbon, carbon-surface transitions, or a combination of both, highlighting the complexity of optical processes in this material.

In order to address these uncertainties and advance our understanding of nanographite, various characterization techniques were employed. In addition to photoluminescence spectroscopy, techniques such as photoluminescence excitation spectroscopy (PLE), UV-Vis spectroscopy, Raman spectroscopy, infrared spectroscopy, and X-ray photoelectron spectroscopy (XPS) were used, all of which provided complementary and enriching information on the optical and structural properties of nanographite. This study significantly contributes to the advancement of knowledge and application of this material in various fields of science and technology

Keywords: graphite nanoparticles, photoluminescence, red shift

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SC1-P018

EFFICIENT PRODUCTION OF NANOGRAPHITE VIA ELECTROCHEMISTRY: RAPID SYNTHESIS

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Within the scope of this study, an electrochemical method designed for the production of nanographite (NG) is presented. This approach represents the synthesis of materials with reduced dimensions with potential applications in various fields, from electronics to energy.

The process is based on the utilization of two graphite rods, sourced from conventional pencils, as electrodes, providing an economic advantage and accessibility to the necessary materials. Additionally, a polarity strategy was implemented, alternating the direction of electric current using an electronic device integrated into the external circuit of the electrochemical cell. This implementation significantly reduced the synthesis time to just 15 minutes, compared to conventional methods that typically require hours of reaction. A mixture with a basic pH and a variable current density was prepared, ranging from 10 to 250 mA/cm².

To evaluate the properties of the obtained nanographite, it was optically characterized using X-ray diffraction (DRX), identifying the preferential directions of graphite. In UV-Vis, two bands were observed, attributed to band gap transitions (HOMO-LUMO) corresponding to conjugated π domains and surface defects. On the Raman side, two characteristic peaks were observed, corresponding to the D and G bands. Complementary

spectroscopies such as photoluminescence, infrared, XPS, and high-resolution transmission electron microscopy (TEM) were performed to complement this study, with particle sizes smaller than 10 nm.

Keywords: graphite nanoparticles, Rapid Synthesis, electrochemical method

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SC1-P020 FLAT-BANDS IN A BILAYER OF PENROSE LATTICES

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Strongly correlated phases in Moiré materials with flat bands in twisted systems, play the main role to explain the superconductivity in Twisted Bilayer Graphene. Decagonal quasicrystals are a type of quasicrystals that has quasiperiodic layers stacked periodically. The Penrose tessellation is the two dimensional most used model to study quasicrystals due to presenting the 5-fold symmetry and quasiperiodicity, as in quasicrystals. In this work, flat bands are found in quasicrystals after a translation and rotation, using the Tight-Binding model. The quasicrystalline phases and confined electronic states rise from rotating two Penrose lattices, which are analysed in detail to understand the emergence of this bands.

Keywords: quasicrystals, flat-bands, bound states

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SC1-P021 ELECTRONIC PROPERTIES OF $\text{FeSe}_x\text{Te}_{(1-x)}$ COMPOUNDS FROM DFT CALCULATIONS

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Iron-based superconductors (IBSC) are extraordinary materials that have surprised the academic community since their discovery in 2008. IBSCs broke a paradigm by showing the existence of superconductors with iron in their chemical composition. Until then, it was thought that it was impossible due to the magnetism properties of this element, making it challenging to form Cooper pairs, an essential ingredient for superconductivity within the BCS theory. Ten years later, Majorana bound states (MBS) in the $\text{FeSe}_{0.55}\text{Te}_{0.45}$ compound were confirmed. This latter constitutes a revolutionary discovery since it was believed previously that these energy modes were exclusive of 1D or 2D materials. Additionally, it was the first time a compound near this material's bulk was detected. This fact could be predicted previously through ab initio calculations that reveal the topology of bands in the electronic structure, which, together with already known properties, postulated it as a strong candidate to house the MBS. These energy modes might be the key to designing more efficient quantum computers and could completely change how the qubit is understood today.

In this work, we study the electronic properties of FeSexTe(1-x) compounds using Density Functional Theory, which employs the van der Waals (VDW) functional form. The structural and electronic properties of these iron-based compounds obtained here agree with previous results when the composition value, x, varies from 0.0 to 1.0. Our results show how the electronic properties are influenced by the composition of IBSC, which can be used to understand the extraordinary properties of these materials.

Keywords: Iron-based superconductor, DFT and VDW functional, electronic properties

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SC1-P022

MULTIFUNCTIONAL ARTHROSPIRA PLATENSIS DERIVED CARBON DOTS USING IN ENVIRONMENTAL REMEDIATION AND OPTOELECTRONIC APPLICATIONS

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Heavy metal pollution in water is a serious risk for human health and living organism. Multicolor fluorescent carbon dots (CDs) exhibit attractive optical properties and wide potential in the environmental remediation. In this work, fluorescent CDs derived from the cyanobacterium *Arthrospira platensis* (Spirulina) have been demonstrated as bio-adsorbent for multiple metal ions. The removal efficiency up to 92% has been achieved. In addition to removal of different metal ions, the CDs after the adsorption process could be used for the optical detection of Cr(VI) in river water. Polymer composites of the proposed algae-based CDs have also been shown as reusable, solid and stable optical sensors towards some selective metal ions as well as white-LEDs. The suggested eco-friendly and sustainable algae-based CDs offer a promising foundation for their efficient application in environmental remediation, optical sensors and optoelectronics.

Keywords: Carbon dots, Heavy metal ions removal, Optical sensor

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SC1-P023

IN SITU/EX SITU SYNTHESIS OF POLYMERIC NANOFIBERS DOPED WITH CARBON QUANTUM DOTS AND THEIR APPLICATION ON THE METHYLENE BLUE DEGRADATION

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CQDs are a relatively new nanomaterial (2004), they present very notable characteristics such as having good solubility in water, biocompatibility, as well as having luminescence properties, among others [1]. On the other hand, most traditional photocatalysts have optical properties that could be improved, and the harvesting of these catalysts has also proven to be a problem. Using nanofibers doped by CQDs can be a possible solution to both arguments. This study presents the preparation and comparison of polymeric nanofibers doped with carbon quantum dots prepared by two methods, and .

The experimental design consists of five phases, these being: 1. Preparation of polymer solutions. 2. Electrospun of samples. 3. Formation of ex-situ samples. 4. Physical characterization. 5. Chemical characterization. The materials were applied for methylene blue (MB) photodegradation. The reaction was monitored by UV-vis.

The obtained nanofiber was analyzed by using different characterization methods such as scanning electron microscopy (SEM), Transmission electron microscopy (TEM), thermogravimetric analysis (TGA), Fourier Transform Infrared Spectroscopy (FTIR) and photocatalytic studies were done to determine the efficiency of the degradation of methylene blue dye.

In general, this study presents another option for the use of CQDs, supported onto an organic nanofiber with potential application as a photocatalyst nanomaterial to reduce water pollution caused by methylene blue.

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Keywords: Carbon Quantum dots, Photocatalytic degradation, Nanofibers

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SC1-P028 DFT CALCULATIONS ON FERROMAGNETIC LAVES PHASE ErAl_2

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In this work, the electronic structure of ErAl_2 Laves phase with a ferromagnetic ordering was study. The total and partial densities of electronic states (DOS and PDOS, respectively) were calculated through density functional theory (DFT) via CASTEP code, using GGA-RPBE framework. The spin polarized DOS and PDOS were used to investigate the magnetic properties of ErAl_2 Laves phases. Also, the contribution of electrons localized at s, p, d, and f for the net magnetic moment was analyzed. The ferromagnetic ordering was simulated considering that only the rare earth element has magnetic moment, and the easy magnetization axis was set along the [001]-direction.

Keywords: Partial and total densities of electronic states, DFT and CASTEP, Laves Phases

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SC1-P029

DFT ANALYSIS OF A CARBON NANOTUBE FOR ADSORPTION OF IBUPROFEN, CARBOXYIBUPROFEN AND HYDROXYIBUPROFEN

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Emerging pollutants such as personal hygiene and pharmaceutical products represent a great risk to our health and the environment. Their presence is well identified in different bodies of water. Ibuprofen and two of its main metabolites (carboxyibuprofen and 2-hydroxyibuprofen) have attracted attention with ibuprofen occupying third place in the world for its use as an anti-inflammatory and painkiller. In this work, an analysis of the adsorption of the mentioned molecules on a carbon nanotube is presented using Density Functional Theory (DFT). We propose this system as a potential alternative for the removal of emerging pollutants in wastewater from domestic use and hospitals. The computational calculations were performed using a chiral carbon nanotube (CNT) (5,6) [1] which was built with the Avogadro program [2], while the ibuprofen molecules and its mentioned metabolites were obtained from the Chemical Entities of Biological Interest (ChEBI) database. The calculations of the Nanotube in its pure form, decorated with silicon and with vacancy as well as the molecules were carried out with B3LYP/6-31G(d)//B3LYP/6-311+G(d,p) for which it was done use of the Gaussian16 program [3]. The energy calculation included ionization potential, electron affinity, HOMO-LUMO energy, as well as Fukui functions. The adsorption energies were determined by subtracting the energy of the molecules and the nanotube from the (NTC)-molecule system. The results demonstrated that a better adsorption was obtained with the nanotube decorated with silicon, reaching the highest adsorption which was for carboxyibuprofen with an energy -38.215 kcal/mol, where the HOMO and LUMO surface analysis can confirm such assertion. Hydroxyibuprofen was adsorbed with an energy of -35.768 kcal/mol, while ibuprofen was adsorbed with a value of -33.258 kcal/mol. The highest ionization potential value corresponds to carboxyibuprofen, (8.707 eV) and the lowest electron affinity -0.625 eV. From this study, we can say that the carbon nanotube (5,6) successfully adsorbs ibuprofen and its metabolites, and therefore these systems would be feasible for the removal of emerging contaminants in water.

Keywords: carbon nanotube, ibuprofen metabolites removal, DFT

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SC1-P030

ELECTRICAL AND THERMODYNAMIC BEHAVIOR OF LATERALLY COUPLED AlGaAs/GaAs QUANTUM DOTS INCORPORATING DONOR IMPURITIES

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In this study, we investigate the electrical and thermodynamic properties of laterally coupled AlGaAs/GaAs quantum dot configurations, each incorporating a single free electron, with a centrally located donor impurity present in one of the quantum dots. We model our system within the framework of effective mass and envelope function approximations to obtain the energy levels and corresponding wave functions from the Schrödinger equation using the finite element method. This approach enables a comprehensive characterization of the electronic energy states and facilitates the computation of the partition function. Utilizing the canonical ensemble approach, we numerically derive the entropy, heat capacity, and average energy of the quantum dot in the presence of electric field. Our results indicate significant transitions of states from atomic-like to very weakly coupled regimes within quantum dot molecules. Furthermore, the heat capacity increases with temperature, highlighting intricate dependencies on environmental conditions. These observations provide valuable insights into the behavior of quantum dot systems, offering profound implications for the design and optimization of nanoelectronic devices.

Keywords: Quantum Dots, Finite Elements Method, Thermodynamics

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SC1-P031

CO₂ ABSORPTION ON CU-DOPED GRAPHENE

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We studied the interaction between a Cu-doped graphene layer and a CO₂ molecule, using DFT, ab-initio calculations and the pseudopotential formalism. We used the software suite Quantum ESPRESSO to perform structural relaxations, and ab-initio molecular dynamics calculations at 300 K. We obtained the PDOS of the different cases considered and performed a Lowdin charge population analysis to characterize the behaviour of the interaction observed. Our results show an interaction between the CO₂ molecule and the Cu-G surface, consistent with a physisorption.

Keywords: DFT, graphene, carbon dioxide

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SC1-P032

DFT CHARACTERIZATION OF HEXAGONAL GRAPHENE QUANTUM DOTS

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Using Density Functional Theory (DFT) and ab initio calculations, we characterized a series of Graphene Quantum Dots (GQDs) using the Quantum ESPRESSO software suite. We obtained their bandgap, their absorption spectra and energy band structure. The DFT calculations were performed using the Generalized Gradient Approximation (GGA) for the exchange-correlation functional, and norm-conserving pseudopotentials. We considered hexagonal GQDs with zigzag configuration. Our results show that the GQDs have a band-gap of around 2.8 eV, which corresponds to a semiconductor behavior and it's congruent to previous results for similar systems. The resulting flat band structure can be optimal for electronics and optoelectronics applications. Our results can be used in a further study on the influences of GQDs edges and the substrate, with potential applications in their production by eco-friendly methodologies.

Keywords: DFT, graphene quantum dots, band structure

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ELECTRONIC AND MAGNETIC CALCULATIONS OF FERROMAGNETIC LAVES PHASE HoAl₂

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The electronic structures of Laves phase HoAl₂ alloys was studied by the density functional theory (DFT). In cubic cell structure (type MgCu₂), the ferromagnetic ordering was simulated considering that the magnetic moments are only carried on by the rare earth atoms. The easy magnetization axis was set along [001] direction. The spin polarized densities of electronic states (DOS) are obtained in order to calculate it magnetic properties. For HoAl₂ alloy, the partial densities of electronic states (PDOS) were used to calculate and analyze the electrons contributions of s, p, d, and f orbitals for the net magnetic moment. Both, DOS and PDOS were simulated by GGA-RPBE framework applying the CASTEP code.

Keywords: Spin polarized DFT, Laves Phases, ferromagnetic ordering

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SC1-P034

EFFECT OF HYDROSTATIC PRESSURE ON ELECTRONIC AND MAGNETIC PROPERTIES BY DFT MODELLING IN ANTIFERROMAGNETIC Fe₅₀Rh₅₀ ALLOY

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Here, a magnetoelastic Fe₅₀Rh₅₀ alloy were studied in a configuration of antiferromagnetic (AFM) ordering along [001] direction under the influence of an external hydrostatic pressure. Spin-polarized calculations were made by density functional theory (DFT) using CASTEP code. A cubic crystal structure (bcc, type CsCl) was constructed with a type-II AFM ordering. Only the Fe atoms were considered to have antiparallel coupling in two identical spin sublattices between successive layers of (111) iron planes, where no spin is established on the Rh atoms. Total (DOS) and partial density of electronic states (PDOS) are calculated. Specifically, the changes in electronic structure induced by an external stress were analyzed. A redistribution of electron population on s, p and d orbitals were observed in DOS and PDOS for high hydrostatic pressures (above 1 GPa). Finally, the stability of crystal structure was analyzed.

Keywords: FeRh magneto-elastic alloy, magneto-caloric alloy, DFT and CASTEP

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SC1-P035

ENHANCEMENT OF OPTICAL PROPERTIES OF CdS COLLOIDAL QUANTUM DOTS BY PREPARING A CORE/SHELL SYSTEM OF CdS/ZnS

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Quantum dots are photoactive nanostructures made of semiconductor materials, and their emission depends on the band gap energy of semiconductor material, with the specific color being related to their size. Due to the wide bandgap energy of CdS (2.42 eV), cadmium sulfide quantum dots (CdS-QDs) can emit within the wavelength spectrum interval from near UV to IR. By the colloidal chemistry technique, CdS can be precipitated in nanocrystals with a wide bandwidth of emission, low intensity and reddish tonality, due to a high defect concentration present on their surfaces which prevents the exploitation of its luminescent properties. One option to passivate surface defects is by the deposition of a semiconductor layer on CdS-QDs surface with a material with higher bandgap energy than CdS, resulting in an improvement in their optical properties, such as luminescence intensity and the targeting of the emission wavelength. Therefore, the preferred approach is to form core/shell systems to passivate the surface, improve the structure of the nanocrystals, and thus enhance their luminescence.

In this work, some advances in the synthesis and optical characterization of CdS-QDs in a core/shell system of cadmium sulfide/zinc sulfide (CdS/ZnS) will be exhibited. The synthesis method employed is based on a "one-pot" approach, including a chemical treatment consists to the deposition on the CdS core surface of a material

with higher bandgap energy material (ZnS shell). Luminescence of samples was activated by thermal treatment under microwave irradiation. The efficiency of this process was evaluated in function of parameters such as temperature, time of thermal treatment and concentration of ZnS layer precursors, by using optical characterization of UV-Vis spectroscopy and photoluminescence. Likewise, measurements of the hydrodynamic radius, Z potential, and electron microscopy analysis were realized.

Keywords: quantum dots, photoluminescence, nanostructures

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SC1-P036 OPTICAL DYE SENSOR WITH CARBON DOTS

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The visual appearance of food significantly influences consumer behavior, prompting the essential use of food coloring to enhance visual appeal. However, numerous studies have revealed harmful effects on both the environment and living beings, including gastric, immunological, neurological issues, and potential cancer risks with excessive consumption. In Mexico, the population is exposed to synthetic food dyes from a young age, as these additives are prevalent in locally consumed products. To address these concerns, this study proposes developing an optical sensor using non-toxic materials to measure dye concentrations. Carbon dots synthesized via the hydrothermal method and doped with various heteroatoms such as phosphorus, nitrogen, and phosphorus-nitrogen were characterized using luminescence spectroscopy and UV-Vis techniques. These carbon dots exhibit stable optical properties in water, enabling sensing based on the reduction in photoluminescence intensity or quenching in the presence of dyes. This research introduces a potential application for effectively detecting dyes and toxic contaminants in commercial products.

Keywords: Sensor, Carbon dots, Dyes

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