

Master in Molecular Nanoscience and Nanotechnology
Master dissertation defense
July 25th, 2025. SS6 Seminar

Confidential

9:00 Javier Alda

Implementation of 2D Materials in Memristive Devices for enhanced Neuromorphic Computing

9:30 Pilar Agustí

Investigating the Ligand Directed Assembly of protein@UiO-66-X

Public

10:00 Beatriz Alba

Comparative Reactivity of Synthesized and Exfoliated MoS₂ Toward Chiral Functionalization

10:30 Jorge Barcia

Tuning ferromagnetism in Fe₃GeTe₂. From bulk to atomically thin crystals

11:00 Pause

11:30 Estrella Parra

Electronic characterization of the quasi-2D antiferromagnet CoNb₃S₆

12:00 Rebeca Sancho

Electrochemical sensors based on core-shell nanoparticles for opioid detection with forensic applications

12:30 Sergio Martínez

Solution Processed Mixed Halide Perovskite Light-Emitting Diodes

13:00 Marta Ubach

Synthesis and characterization of piezoelectric materials for energy harvesting

Master's Thesis

Master in Molecular Nanoscience and Nanotechnology

2024-2025

Implementation of 2D Materials in Memristive Devices for enhanced Neuromorphic Computing



Javier Alda Gómez

Master Thesis co-supervised by:

Dr. Ramón Torres Cavanillas

Prof. Eugenio Coronado Miralles

July 2024

Investigating the Ligand Directed Assembly of protein@UiO-66-X

Master's Thesis in Molecular Nanoscience and Nanotechnology

2024/2025

M^a del Pilar Agustín Mahiques

Directed by:

Dr. Jana Maren Glatz

Prof. Mónica Giménez Marqués

July 15th, 2025



VNIVERSITAT
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EXCELENCIA
MARIA
DE MAEZTU

Master's Thesis

**Comparative Reactivity of
Synthesized and Exfoliated MoS₂
Toward Chiral Functionalization**

Author

Beatriz Alba Sangrós

Supervisor

Alicia Forment Aliaga

Master of Molecular Nanoscience and Nanotechnology

Abstract

This work focuses on the functionalization of molybdenum disulfide synthesized *via* two distinct approaches: a bottom-up method through hydrothermal synthesis (**HT-MoS₂**) and a top-down method based on chemical exfoliation (**ce-MoS₂**). To achieve this, two different molecules were employed: **cysteine**, a chiral amino acid capable of forming covalent bonds with the MoS₂ surface, and **rac-[Cr(dqp)₂]³⁺**, a cationic chromium(III) complex that interacts primarily through electrostatic forces. Indeed, a clear reactivity difference is achieved, as HT-MoS₂ catalyses the oxidation process of cysteine obtaining cystine, while ce-MoS₂ can be directly used without oxidation problems.

The study aims to compare the structural and electronic changes induced by each type of functionalization, relative to the non-functionalized materials, and to assess how the synthesis method (HT vs. exfoliated) influences the formation and behaviour of the resulting composites.

Resum

Aquest treball se centra en la funcionalització del disulfur de molibdè sintetitzat mitjançant dues aproximacions distintes: un mètode *bottom-up* mitjançant síntesi hidrotermal (**HT-MoS₂**) i un mètode *top-down* basat en l'exfoliació química (**ce-MoS₂**). Per a dur-ho a terme, s'han emprat dues molècules diferents: la **cisteïna**, un aminoàcid quiral capaç de formar enllaços covalents amb la superfície del MoS₂, i el complex catiònic de crom(III) **rac-[Cr(dqp)₂]³⁺**, que interactua principalment per forces electrostàtiques. De fet, s'aconsegueix una clara diferència de reactivitat, ja que HT-MoS₂ catalitza la reacció d'oxidació de la cisteïna per a obtenir cistina, mentre que ce-MoS₂ es pot emprar directament sense problemes d'oxidació.

L'estudi té com a objectiu comparar els canvis estructurals i electrònics induïts per cada tipus de funcionalització, respecte als materials no funcionalitzats, i avaluar com influeix el mètode de síntesi (HT vs. exfoliat) en la formació i el comportament dels compostos resultants.

UNIVERSITY OF VALENCIA

MSC IN MOLECULAR NANOSCIENCE AND
NANOTECHNOLOGY

Tuning ferromagnetism in Fe_3GeTe_2 from bulk to atomically thin crystals.



Jorge Barcia Rodríguez

Supervised by:

Prof. Efren Navarro-Moratalla
Jose Joaquín Pérez Grau

July 2025

Abstract

In this work we report an experimental investigation of the ferromagnetic phase in Fe_3GeTe_2 (FGT), a metallic van der Waals magnet, going from bulk crystals down to atomically thin flakes. By mechanical exfoliation and hBN encapsulation, we fabricated Hall devices to probe both electrical and magnetic transport between 4.5 K and 300 K. The Curie temperature steadily drops from 220 K in thick samples to 110 K in four-layer structures, coinciding with a crossover from metallic conduction to a two-dimensional hopping insulator. Finally, we assess two routes for electrical modulation, electrostatic gating and ferroelectric coupling via CuInP_2S_6 heterostructures, and no clear magnetic response was observed, attributed to strong carrier screening in FGT and the difficulties of fabricating such complex devices. These results point the way to improving the electrical control of 2D magnets in future spintronic devices.

2025

Electronic characterization of the quasi-2D antiferromagnet CoNb_3S_6



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Student: Estrella Parra Guillén

Supervisor: Dra. Carla Boix Constant

Master Thesis in Molecular Nanoscience and Nanotechnology

July 2025

Abstract.

Two of the most studied magnetic phases present in magnetic materials are ferromagnetism (FM) – showing net magnetization due to spin alignment and time-reversal symmetry breaking – and antiferromagnetism (AFM) – exhibiting compensated magnetic moments and zero net magnetization. Recently, a new phase named *altermagnetism* has been theoretically proposed, combining spin-split band structures (typical of FM) with a compensated spin order (associated with AFM ordering)^{1,2}.

This work focuses on CoNb_3S_6 , a quasi-2D collinear antiferromagnet with a chiral lattice and Néel temperature around 28 K. This system was theoretically proposed as an altermagnetic candidate, showing signs of time-reversal symmetry breaking and anomalous Hall effect – features consistent with a FM behaviour, not AFM as originally proposed for the material³. To further investigate its predicted altermagnetic nature, we synthesize bulk crystals of CoNb_3S_6 using solid-state chemistry techniques – in particular, the chemical vapour transport method – and perform a detailed characterization of its structural, chemical and magnetic properties, both in the bulk form and in the exfoliated flakes. Single-crystal X-ray diffraction and energy dispersive X-ray spectroscopy will be used to confirm phase purity and crystallinity, atomic force microscopy will allow the determination of the thickness of the obtained thin layers, and a superconducting quantum interference device will provide an insight into its magnetic ordering. We also report for the first time the Raman spectra of the system, where an in-plane anisotropy has been detected by using polarised incident light. Magneto-transport measurements will be performed to further characterize the electronic response of the material and to investigate its potential as an altermagnetic candidate.

In this context, the study of theoretically predicted altermagnetic candidates would contribute to a broader understanding of this novel magnetic phase from a more fundamental point of view, where the family of intercalated transition metal dichalcogenides – to which the system CoNb_3S_6 belongs to – show a big potential in the field of spintronics. Moreover, its layered nature may contribute, in the long term, to the study of this phase at the two-dimensional limit, enabling their integration in miniaturized devices for developing new technological applications.

Master Thesis

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**Electrochemical sensors based on core-shell
nanoparticles for opioid detection
with forensic applications**

Rebeca Sancho Barbero

Supervised by Dr. Joaquín Soriano López

July 2025

Abstract

The increasing prevalence of opioid-related incidents underscores the urgent need for rapid and reliable detection methods. In this work, we develop an electrochemical sensor based on a glassy carbon electrode (GCE) modified with tailored inks based on nanomaterials with high surface area and electrocatalytic activity for the detection of diacetylmorphine (heroin) and codeine. The nanomaterials employed include gold nanoparticles (AuNPs) and iron oxide nanoparticles ($\text{Fe}_3\text{O}_4\text{NPs}$), both coated with Prussian Blue Analogues (PBA) to form Au@PBA and $\text{Fe}_3\text{O}_4\text{@PBA}$ core@shell structures. The core@shell nanoparticles were characterised through surface analysis techniques to confirm their morphology and composition. Furthermore, the modified electrodes were characterised through electrochemical impedance spectroscopy (EIS) to assess charge transfer resistance before and after nanoparticle coating, as well as cyclic voltammetry (CV). The main target is to employ the sensors for the detection of opioids using differential pulse voltammetry (DPV). While the development of a fully portable sensor is beyond the scope of this study, our findings lay the groundwork for future advancements in on-site forensic applications. This research highlights the importance of material characterisation in sensor development and its potential forensic and biomedical applications. The proposed sensor offers high sensitivity, selectivity, cost-effectiveness, and rapid analysis, making it a promising alternative to conventional, time-consuming techniques.

Resumen

El creciente aumento de incidentes relacionados con los opioides evidencia la necesidad urgente de métodos de detección rápidos y fiables. En este trabajo desarrollamos un sensor electroquímico basado en un electrodo de carbono vítreo (GCE) modificado con tintas formuladas a partir de nanomateriales con alta superficie específica y actividad electrocatalítica para la detección de diacilmorfina (heroína) y codeína. Los nanomateriales empleados incluyen nanopartículas de oro (AuNPs) y nanopartículas de óxido de hierro ($\text{Fe}_3\text{O}_4\text{NPs}$), ambas recubiertas con análogos de Azul de Prusia (PBA) para formar estructuras núcleo-cáscara Au@PBA y $\text{Fe}_3\text{O}_4\text{@PBA}$. Las nanopartículas núcleo-cáscara se caracterizaron mediante técnicas de análisis superficial para confirmar su morfología y composición. Además, los electrodos modificados se caracterizaron mediante espectroscopía de impedancia electroquímica (EIS) para evaluar la resistencia de transferencia de carga antes y después del recubrimiento, así como mediante voltamperometría cíclica (CV). El objetivo principal es emplear estos sensores para la detección de opioides mediante voltamperometría de impulsos diferenciales (DPV). Aunque el desarrollo de un sensor completamente portátil queda fuera del alcance de este estudio, nuestros resultados sientan las bases para futuros avances en aplicaciones forenses in situ. Esta investigación subraya la importancia de la caracterización de materiales en el desarrollo de sensores y su potencial en ámbitos forense y biomédico. El sensor propuesto ofrece alta sensibilidad, selectividad, bajo coste y un análisis rápido, lo que lo convierte en una alternativa prometedora a las técnicas convencionales, más laboriosas y prolongadas.



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Master's Thesis

Solution Processed Mixed Halide Perovskite Light-Emitting Diodes

Author

Sergio Martínez Saiz

Supervisor

Daniel Tordera Salvador

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Abstract

Lately, n-type semiconductor hybrid organic-inorganic perovskites have become promising materials for light-emitting diodes (LEDs) by virtue of their excellent optical properties and the possibility of tuning their emission colour with ease by changing their chemical composition. By combining additive-based nanocrystal pinning (A-NCP) and a passivator molecule like (4-(9H-carbazol-9-yl)butyl) phosphonic acid (4PACz), solution-processed perovskite particles can be converted from n- to p-type semiconductors leading to outstanding performance in green LEDs reaching a maximum luminance of $1.1 \cdot 10^6 \text{ cd} \cdot \text{m}^{-2}$ and a maximum External Quantum Efficiency (EQE) of 28.4%. Despite this, there is still no report of this approach being applied to perovskites with different halide compositions. This work demonstrates the possibility of using A-NCP and 4PACz to fabricate efficient PeLEDs with the composition $(\text{FA}_{0.80}\text{MA}_{0.10}\text{GA}_{0.10})_{0.87}\text{Cs}_{0.13}\text{PbX}_3$ ($\text{X} = \text{Cl}^-$, Br^- , I^- mixtures). The structural properties of the films were studied through X-ray diffraction, scanning electron microscopy, and energy dispersive X-ray spectroscopy, which confirmed that perovskite structures were formed and their composition. The LEDs' properties, such as the colour emission of the device or their EQE, were assessed. Their emission could be tuned from blue LEDs towards near infrared (NIR), reaching a remarkable EQE of 25.97% in mixed bromide-iodide LEDs.

Resumen

Últimamente, los semiconductores tipo n, como las perovskitas orgánicas-inorgánicas híbridas se han convertido en materiales prometedores para diodos emisores de luz (LEDs) en virtud de sus excelentes propiedades ópticas y la posibilidad de cambiar su colour de emisión con facilidad modificando su composición química. Combinando la fijación de cristales mediante aditivos (A-NCP) y una molécula pasivadora como el ácido (4-(9H-carbazol-9-il)butil) fosfónico (4PACz), partículas de perovskita procesadas mediante disolución se puede cambiar de semiconductores tipo n a tipo p, dando lugar a un funcionamiento sobresaliente en LEDs verdes, alcanzando una luminancia máxima de $1.1 \cdot 10^6 \text{ cd} \cdot \text{m}^{-2}$ y una Eficiencia Cuántica Externa (EQE) de un 28.4%. Sin embargo todavía no hay ningún reporte de este método siendo aplicado a perovskitas con diferentes composiciones de haluros. Éste trabajo demuestra la posibilidad de usar A-NCP y 4PACz con el fin de fabricar PeLEDs cuya perovskita tiene una composición de $(\text{FA}_{0.80}\text{MA}_{0.10}\text{GA}_{0.10})_{0.87}\text{Cs}_{0.13}\text{PbX}_3$ ($\text{X} = \text{Cl}^-$, Br^- , I^- y mezclas). Las propiedades estructurales de los films fueron estudiados mediante difracción de rayos X, microscopía electrónica de barrido y espectroscopia de rayos X de energía dispersiva, que confirma que la perovskita se ha formado. Las propiedades de los LEDs, como el color de emisión del dispositivo o el EQE han sido evaluadas. Su emisión se ha podido modificar desde LEDs azules hacia el infrarrojo cercano (NIR) alcanzando un EQE extraordinario de 25.97% en LEDs con una mezcla de bromuro y yoduro.

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**SYNTHESIS AND CHARACTERIZATION
OF PIEZOELECTRIC MATERIALS
FOR ENERGY HARVESTING**

MARTA UBACH
FERNÁNDEZ

Thesis supervised by
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University of Valencia, July 2025