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Book of Abstracts

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Hydrothermal synthesis and characterization of h-WO3 pure and doped with transition metal ions

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In the field of hydrogen (H2) production, the fabrication of the materials with high pseudocapacitance is fundamental. Existing electrodes for this goal are mainly based on platinum making them very expensive. Therefore, the design and develop of nanomaterials with high pseudocapacitance to replace platinum electrodes become an essential task.
Tungsten trioxide in hexagonal phase (h-WO3) is a good candidate to solve this issue because of its high electrochemical stability in acidic environment, good resistance to electrochemical corrosion, low cost and toxicity and earth abundance. However, when stoichiometric it suffers of a poor electron conductivity, which can be enhanced by metal-doping, which in principle changes also their electrochemical properties.
In the present work, we present recent results of h-WO3 synthesis pure and doped by transition metals (WO3-Me) for electrocatalytic applications.
h-WO3 and h-WO3:Me have been fabricated by hydrothermal method ensuring several advantages such as simplicity of the procedure, high efficiency, low costs and good reproducibility of the samples. For doping, following metals have been used Co, Cr, Ni, Mo, Ti. The doping concentration was M[Me]/M[WO3] = 5% for all used metals.
Structure, electronic and optical properties of the h-WO3 samples have been studied by SEM, TEM, BET, XRD, FTIR, Raman, and diffuse reflectance methods.
Electrochemical properties of the h-WO3 samples have been studied by cyclic voltammetry. Specific capacity of each sample was calculated. Comparative analysis of doping to structure, optical and electrochemical properties has been discussed. Samples with the higher stability and higher specific capacitance, those doped with Ti and Mo, represent good candidates to develop new electrodes suitable for applications in the field of H2 production.

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Investigation of polymorphism in organic luminophores

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Synthesis of organic nanomaterials requires precise control on many technological parameters. For instance, drying and crystallization speed define conformation of the chemical structure and main fundamental properties of the organic luminophores. Deviation from the fabrication protocol results in forming of polymorphous structures with same chemical composition but different structural, electronic and optical properties.
In the present work, 1-(2-(3,6-dimethyl-9H-carbazol-9-yl) benzyl) pyridin-1-ium methanesulfonate

(KL1421) has been crystallized with different drying rates. Structure and electronic properties of the polymorphous samples have been studied by NMR, XRD, FTIR and Raman spectroscopy. Investigation of optical properties by photoluminescence showed changes of the quantum yield and emission peak position. Activation energies have been studied by temperature quenching of the photoluminescence. Correlation between structure, optical and technological parameters have been proposed.

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Photochemical sensor application of Salan-type ligands TFA salts for Cu^{2+} and Fe^{3+} detection in aqueous media

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Ligands with chelating properties, such as Schiff bases, imines, and Salan-type ligands, are promising materials for photochemical sensors of metal ions, which require good sensitivity and selectivity. The ability of such ligands to host metal ions in their molecular structure and specific optical properties, such as high intensity photoluminescence, create new opportunities to define metal ion concentration in aqueous media by optical methods with fairly high accuracy. In addition, the structure of the ligand could be chemically tuned according to the requirements of the sensor. [1]
In this work, the sensitivity and selectivity of Salan ligands TFA salts were investigated by photoluminescence (PL) and transmittance (TM) methods.
Salan ligands were synthesized in salt form to make them soluble in water and alcohols. For sensor testing, the ligands and metal salts were dissolved in ethanol at a concentration of 100 mkM/L.
Sensor testing was performed in a home-built system with a quartz cuvette equipped with a magnetic stirrer, Fiber optic spectrometer, system of lenses and filters, Fiber optic cables, and a portable 325 nm UV light source with detector.
During the measurement steady-state PL and TM spectra were saved after each metal ion probe. The kinetics of local PL and TM peaks were recorded. The sensitivity to Cu^{2+} and Fe^{3+} ions in sub micromolar range was observed. Complex formation of ligand with Cu and Fe was proofed by FTIR. Mechanisms of interaction were proposed, main sensors parameters were calculated.

Keywords: photochemical sensors, metal ions detection, chelators

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Production of core-shell Metal Organic Frameworks (MOFs) Hybrids for Sensing Applications

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MOFs are top notch candidates for sensing applications due to their high porosity, large surface area, and highly exposed surface sites, which are prone to specific interactions with target molecules, ions or gases. MOFs are produced by the self-assembly of multidentate organic ligands connecting with multivalent metal nodes through strong coordination interactions. The unlimited combinations of metals and ligands allow the design and preparation of ad-hoc structures. Surface chemistry and microstructure (i.e. exposed facets, surface defects, polarity) have a significant impact on surface and bulk interaction process. The MOF flexibility for pre- and post-processing can be exploited to enhance the performance toward sensing applications, particularly by combining with organic and inorganic materials to produce composite materials. Polymers, metal oxides, metal nanoparticles, carbon nanotubes, quantum dots and GRMs are the most commonly used materials for the preparation of MOF composites and hybrids 1. In this work, core-shell hybrid materials obtained allowing the MOF structure to growth onto the surface of zinc oxide nanoparticles are reported. In the synthesis strategy adopted here, zinc oxide serves as both the core-shell structure and the metal source for the growth of MOF structures. Zinc-based zeolitic imidazolate frameworks (ZIFs) are chosen for the MOF shell due to their robust porosity, resistance to thermal changes, and chemical stability. Different types of imidazole-based linkers have been explored to fabricate ZIF-based hybrids (Fig.1).

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The obtained materials have been full characterized from the morphological, structural and textural points of view highlighting the instauration of synergistic effects between the hybrid components. A selection of the produced materials has been also tested for the detection of metal ions in solution.

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Photothermal Targeted Ablation of Melanoma Using MXene-PDA-anti-CEACAM1 Complex

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We examine MXenes as optical absorption agents for photothermal treatment (PTT) in this study. To ensure targeted delivery of MXenes, we linked them to the monoclonal anti-CEACAM1 antibody (mAb).
Our study uses an NIR-I laser to evaluate the targeted photothermal effect in vitro and to offer biological characterization of the MXene-anti-CEACAM1 antibody combination. After polydopamine (PDA) of varying thicknesses was added to delaminated Ti3C2Tx MXenes, human anti-CEACAM1 mAb was immobilized. The complex's specificity, affinity, biocompatibility, and selective photothermal ablation were all examined.
Our findings show that after 4 and 24 hours of incubation with various melanoma cell types and keratinocytes, the MXene-anti-CEACAM1 complex and its constituent parts (MXenes, MXene-PDA, and anti-CEACAM1 mAb) do not exhibit any cytotoxicity. Our findings show that thickening the PDA layer decreases photothermal conversion but has no effect on biocompatibility, specificity, or affinity. Modes of laser irradiation were chosen experimentally to safely affect non-targeted cells while also successfully influencing the complex. When target cells are loaded with MXene-PDA-anti-CEACAM1 mAb complexes, highly selective tumor cell ablation utilizing near-infrared irradiation

(NIR) is seen.
We concluded that the use of a combination of MXene-anti-CEACAM1 mAb for selective PTT of tumor cells has significant potential for creating a new model of targeted treatment of melanoma.
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Keywords: MXenes, cancer treatment, targeted photothermal ablation

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Harnessing Hybrid Nanoarchitectures for Next-Generation Photoelectrochemical Energy conversion

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Abstract
The global energy crisis and environmental concerns have intensified the search for sustainable and renewable energy sources. Among various strategies, solar-assisted water splitting has emerged as a promising approach for producing clean hydrogen fuel. However, the efficiency of this process is largely dependent on the development of advanced materials that can effectively absorb sunlight, generate charge carriers, and minimize recombination losses. One-dimensional semiconductor nanowires and two-dimensional conductive materials offer a unique combination of properties that can significantly enhance charge transport and interfacial charge separation 1.

In this study, we investigate the synergistic effects of zinc oxide (ZnO) nanowires and layered Ti3C2 (MXene) as hybrid photoelectrodes for solar-driven hydrogen production. ZnO, known for its wide bandgap (3.37 eV) and excellent stability in aqueous environments, suffers from rapid charge carrier recombination, limiting its efficiency in photocatalysis. To overcome this challenge, the integration of ZnO with MXene an emerging class of two-dimensional transition metal carbides offers a promising strategy due to its high electrical conductivity, excellent charge transport properties, and tunable surface chemistry23. The optimized ZnO/MXene exhibited the highest solar-to-hydrogen (STH) efficiency compared to pure ZnO, highlighting the critical role of interfacial engineering in maximizing solar energy conversion. By leveraging the combined advantages of semiconductor nanowires and highly conductive nanosheets, this work provides valuable insights into the design of next-generation photoelectrodes for scalable and efficient hydrogen production.

Keywords: MXene; photoelectrochemical water splitting; composite photoelectrode; photocatalysis; charge separation

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Biocompatibility of MXenes: influence of flake size and surface terminations

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The groundbreaking discovery of graphene in 2004 sparked a surge of interest in the search for novel two-dimensional (2D) materials. Among these, MXenes, first identified by Yury Gogotsi and Michel Barsoum at Drexel University in 2011, have emerged as particularly promising. To date, more than fifty MXene variants have been synthesized, with many more predicted through theoretical models. Over the past decade, MXenes have demonstrated remarkable versatility, with potential applications spanning lithium and sodium-ion batteries, electrocatalysis, optoelectronics, flexible electronics, and various biomedical fields, including cancer treatment, antimicrobial therapies, immunomodulation, targeted drug delivery, and tissue regeneration.
With the growing interest in MXenes for biomedical applications, it is imperative to thoroughly investigate their biocompatibility to ensure both safety and efficacy. In addition, evaluating their biosafety is critical, given the potential environmental risks that may arise from widespread use. Despite numerous studies, defining consistent toxicity profiles for MXenes remains a challenge. This difficulty largely stems from variability in experimental outcomes, even when similar MXene compositions are analyzed. Such inconsistencies are often attributed to differences in chemical purity, levels of oxidation, and the characteristics of surface terminations (Tx) in the materials.
To clarify the influence of MXene properties on biological systems, we conducted an in-depth assessment of how flake size, surface terminations, and oxidation states affect cell viability and metabolic activity over varying exposure durations. Our research revealed a clear connection between the dimensions of Ti_3C_2, V_2C, and Nb_2C MXene flakes, their surface chemistry, and the corresponding cellular responses. These responses encompass the uptake of MXene particles by cells, as well as the activation of pathways leading to apoptosis, necrosis, and genotoxicity. The results emphasize that fine-tuning the structural and chemical features of MXenes is crucial for tailoring their performance in biomedical contexts.

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Keywords: MXenes, biocompatibility,

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Enhanced Antibacterial Activity of MXenes Through Photothermal Therapy (PTT) Compared to Conventional Antimicrobial Approaches

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MXenes, a novel class of two-dimensional (2D) materials, have garnered significant attention due to their remarkable antibacterial properties. Among them, $Ti_3C_2T_x$ stands out as the most extensively studied representative, demonstrating notable antibacterial activity 1. The antimicrobial effects of MXenes are primarily attributed to several key mechanisms: oxidative stress, photothermal therapy,

and physical disruption of bacterial membranes [2]. They also exhibit strong photothermal conversion efficiency, enabling effective bacterial eradication through localized heating under near-infrared (NIR) light exposure [3]. These unique characteristics position MXenes as promising candidates for the development of next-generation antibacterial therapies and coatings.

This study investigates the antibacterial efficacy of various MXene formulations (Ti_3C_2, V_2C and Nb_2C) against S. aureus and E. coli using diffusion-based and dilution-based assays. While disk diffusion and drop dilution methods did not reveal significant antimicrobial activity, broth microdilution, and time-kill kinetics assays demonstrated a concentration-dependent antibacterial effect. Time-kill kinetics assays revealed MXene-mediated bacterial reduction over 4 and 24 hours, confirming time- and concentration-dependent effects. Spectrophotometric analysis, however, was limited due to interference from MXene-induced turbidity, restricting quantitative assessments at higher concentrations. Furthermore, biofilm inhibition was investigated using the crystal violet assay, which demonstrated that MXene-integrated membranes impeded bacterial adherence only at concentrations of 2000 μg/mL.

At concentrations ranging up to 200 μg/mL, MXenes exhibited considerable cytotoxicity to mammalian cells, limiting their potential for direct use as antimicrobial agents. To address this challenge, photothermal therapy (PTT) was explored as a viable strategy. Upon exposure to near-infrared (NIR) laser irradiation, MXenes effectively converted light into heat, resulting in bacterial membrane disruption and microbial death. This approach enabled the use of significantly lower MXene concentrations (50–100 μg/mL), which have been reported to be biocompatible. Membrane integrity assays, including propidium iodide uptake and colony-forming unit (CFU) quantification, confirmed the structural damage caused by this treatment. These findings suggest that MXene-based PTT holds great promise as an antibacterial strategy, overcoming the limitations associated with high MXene concentrations. The study underscores MXenes as promising candidates for next-generation antimicrobial materials, with an emphasis on optimizing their stability and dispersion in biological media for broader applications.

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