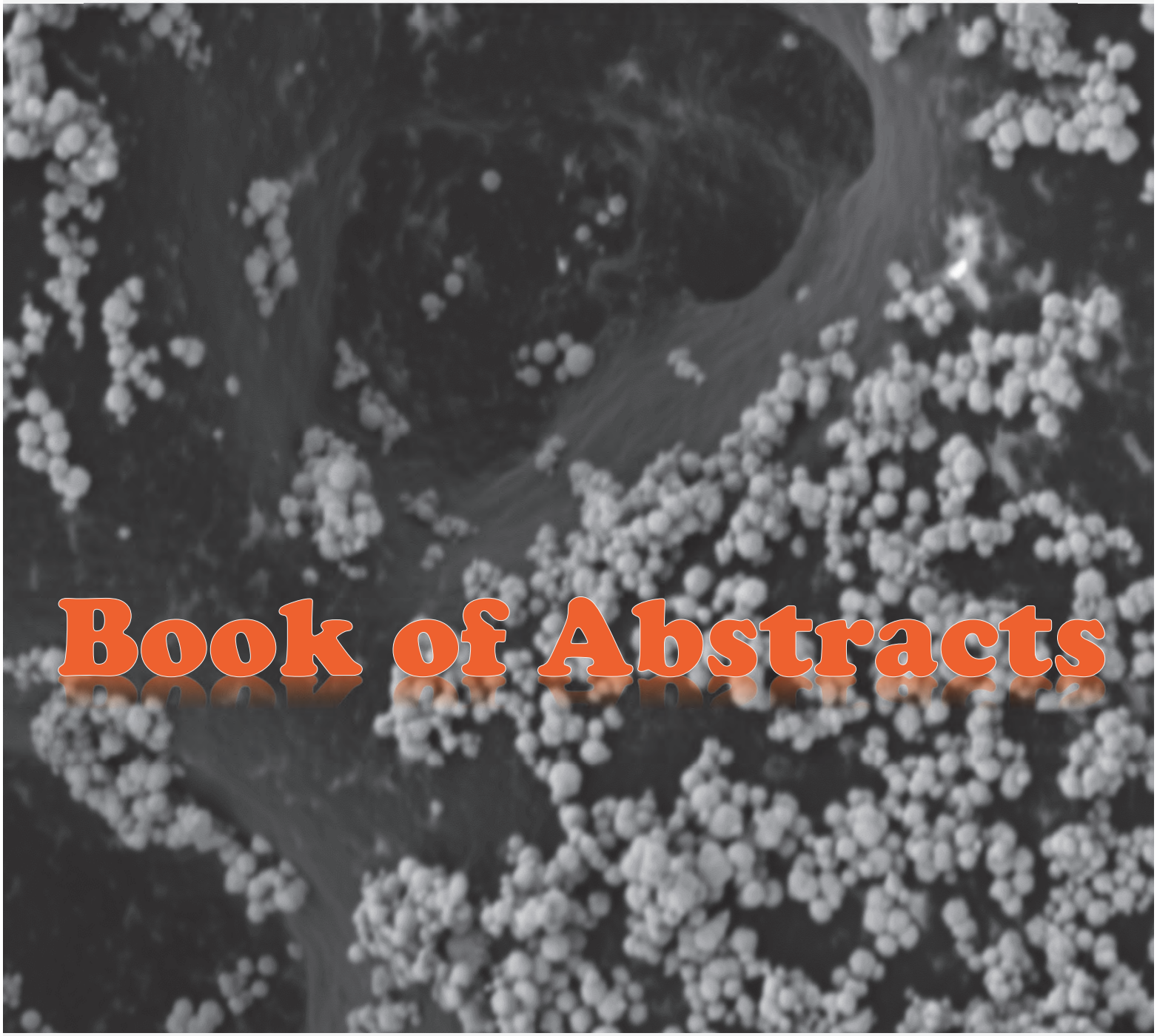
The 3rd International Workshop Advances on Photocatalysis including Environmental and Energy Applications AdvPhotoCat-EE 2021



Book of Abstracts

Organizers

IMT Bucharest Romania

Hellenic Mediterranean University

Center of Materials Technology and Photonics, Crete Greece

AdvPhotoCat-EE2021

In the framework of **Project** PN-III-P1-1.1-TE-2019-0594 **"Novel nanostructured composite-membranes for enhancement of photocatalytic processes in water purification "**Grant of the Romanian National Authority for Scientific Research, CNCS – UEFISCDI

The 3rd International Workshop Advances on Photocatalysis including Environmental and Energy Applications AdvPhotoCat-EE 2021

Book of Abstracts

ONLINE

June 28-29, 2021

Organizing committee board

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Contents

About

The 3rd International Workshop Advances on Photocatalysis including **Environmental and Energy Applications AdvPhotoCat-EE 2021**, that will take place **ONLINE,** on **June 28-29, 2021**, focuses on the experimental and theoretical aspects of photocatalysis and its real life applications like environmental and energy. The scope is to open an extensive discussion on the scientific areas involved between academia, research and industry.

The workshop will try to review the recent advancements on photocatalytic processes and their application to environmental remediation, solar fuels production and energy, green chemical synthesis, etc and open discussions about possible common activities and collaborations between the participants.

On behalf of the Organizing Committee, we are pleased to invite you to this event, that will take place ONLINE**,** on **June 28-29, 2021.**

The event will feature invited talks, oral presentations and online poster exhibition, in parallel to the talks. Posters may be optionally presented as 3 minutes oral presentations, while, discussions sessions on the posters will be also included. The workshop participants will have the option of publishing their scientific contributions in a ***Special Issue of "Surfaces and Interfaces" Elsevier Journal (IF 3.72)***

The proposed topics are:

- Basic research on photocatalysis
- Photocatalytic materials
- Photoelectrochemistry
- Photocatalysis in life sciences
- Green chemistry
- Modern trends in clean energy production and storage
- Modern trends in environmental remediation and protection.

Previous editions:

Facebook https://web.facebook.com/photocatalysisworkshop and
Facebook group https://web.facebook.com/groups/407479032768229

1st International Workshop Advances on Photocatalysis, **AdvPhotoCat2015** July 6 – 8, 2015, Universitatea Alexandru Ioan Cuza din Iași, Romania

The 2nd International Workshop Advances on Photocatalysis – AdvPhotoCat-E 2017 July 14-16, 2017, CEMATEP – Technical Educational Institute of Crete, Heraklion, Crete, Greece

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INVITED PRESENTATIONS

Antimicrobial/antiviral applications of transparent photocatalytic coatings

Raffaella Moro (*) (X), Angelo Del Favero (*), Pierluigi Biasiolo (**), Gian Luca Guerrini (*)(***) (X)
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Infections caused by microorganisms such as bacteria and viruses are a leading cause of disease and death worldwide. They can be transmitted especially in indoor environments both through respiratory droplet and contact routes. Although the most recent SARS COv-2 virus studies that have been carried out in the last year seem to attribute greater importance to the transmission of viral particles through the respiratory tract and therefore due to the presence of aerosols and droplets in the confined environments, the need to guarantee the cleaning, sanitation and sanitization of surfaces, which are also means of transmission of pathogens, remains fundamental, especially in hospitals but generally in public places.

Due to the COVID 19 pandemic, biological risk has thus become a new priority in the management of indoor environments which must therefore be sanitized through the adoption of clear and regular operating protocols.

Surfaces are sanitized mainly using chemical disinfectants which are effective but have an instant and not a lasting benefit. Therefore, it becomes important to propose protocols where photocatalytic products are used in order to guarantee a long duration and efficacy. In this case, we will reduce considerably tthe use of large quantities of chemical products that have a negative impact on the environment (pollution), and on the occupants wellbeing.

Transparent coatings that do not change the surface appearance and colour of the substrates, adhere and adapt to all curves, are among the most easily applicable photocatalytic products with a relatively low economic impact.

The other surface coating materials are white, coloured paints or varnishes, or they are rigid flat products (tiles, panels) generally usable for new projects or for renovations, with costs per square meter often not exactly negligible (beyond the specific photocatalytic performances that are provided). They are also active inside buildings in both natural and artificial light conditions.

Finally, photocatalytic products must guarantee efficacy, long life against microorganisms and their performances must be measurable and monitorable over time, through certified tools that quantify the presence of microorganisms on surfaces (such as the bio-luminometer).

The treated surfaces can be vertical and of various types of materials (walls, partitions, glass, concrete, fabrics) and other in direct contact with the people (tables, chairs, worktops, work tools).

In this work, an example of a protocol proposed for the photocatalytic treatment of indoor environments will be presented and some examples of recently completed applications in different sectors (for example: hospitals, schools, airport infrastructures, offices, shops, medical centres, ships).

Homogeneous photocatalytic reduction of CO2

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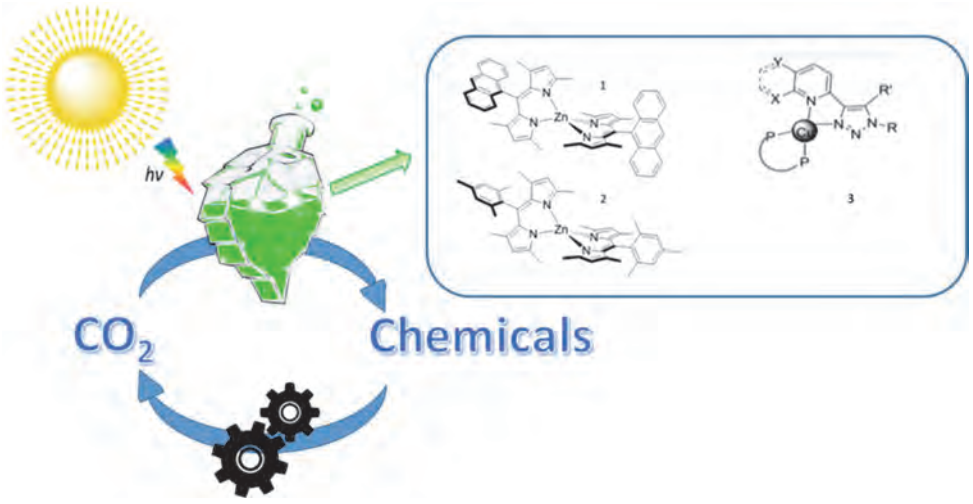
Solar energy is the only renewable and carbon-neutral energy source of sufficient scale to replace fossil fuels.[1] The direct conversion of light into chemical bond energies has the advantage over photovoltaics to be able to store large amount of energy in form of chemicals. Important milestones have been recently achieved on artificial photosynthesis,[1b-1c] nevertheless in terms of applicability, these photosensitizers should be easily available and cost-effective, thus, earth-abundant materials are highly desired.[2-3] New bis(dipyrrinato) Zn(II) complexes[3] and new heteroleptic Cu(I) complex (mononuclear and multinuclear), obtained by modification of the diimine ligand, based on substituted 1,2,3-1H-triazole,[2] are presented. We explore their photophysical and electrochemical properties, revealing that these metal complexes possess an unordinary high photoluminescence quantum yield. Further strategies to lower non-radiative constants will be discussed, as the use of mesoporous silica.[4] Finally, some experiments on photoreduction of carbon dioxide are presented.[5]



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New insights into Nanomaterials for Photocatalytic Applications

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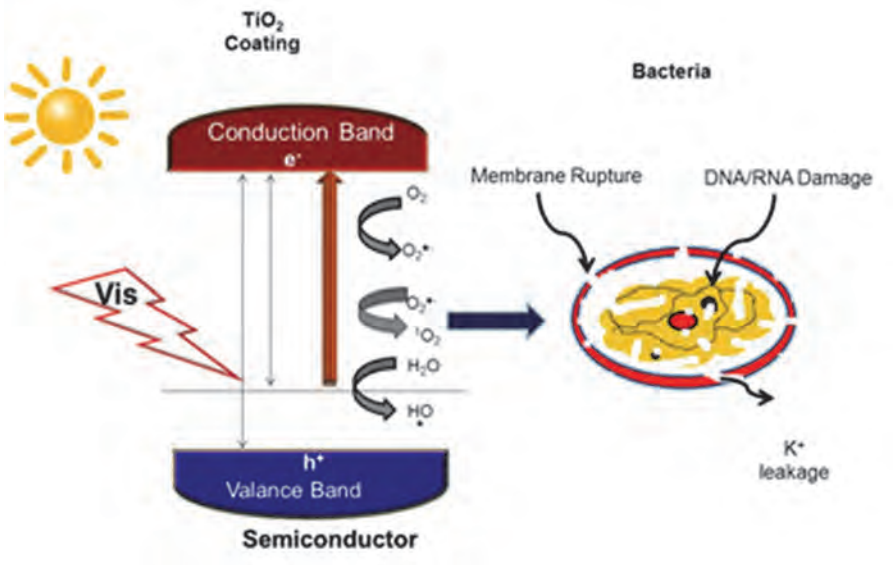
Functional semiconductor nanomaterials which could show photocatalytic activities under the natural light (typically >400 nm) is preferred for industrial applications. As part of a program to develop efficient surface coatings, our investigations were focused in the development of novel catalysts for anti-bacterial applications. Anatase phase of TiO_2 thermally stable up to the sintering temperature of the substrates (*e.g.*, bathroom tiles) is most desirable for building materials applications. Anatase phase thermal stability at elevated temperatures is one of the requirements for making such coatings on industrial scale. The preparation of novel photo-catalytic materials by modifying the band-gap using various dopants such as F, S, N and C will be discussed.



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Photocatalysis and virus: an industrial perspective

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The ongoing pandemic situation due to the spread of the SARS COv-2 virus has created considerable applicative interest for photocatalysis technology for improving indoor air quality, with reference to microorganisms.

In this talk, the main mechanisms that can be exploited for the inactivation of viruses and for their killing – in other words, for an effective sanitization of the environments – are briefly described and the main results obtained in terms of research and product development are also reported.

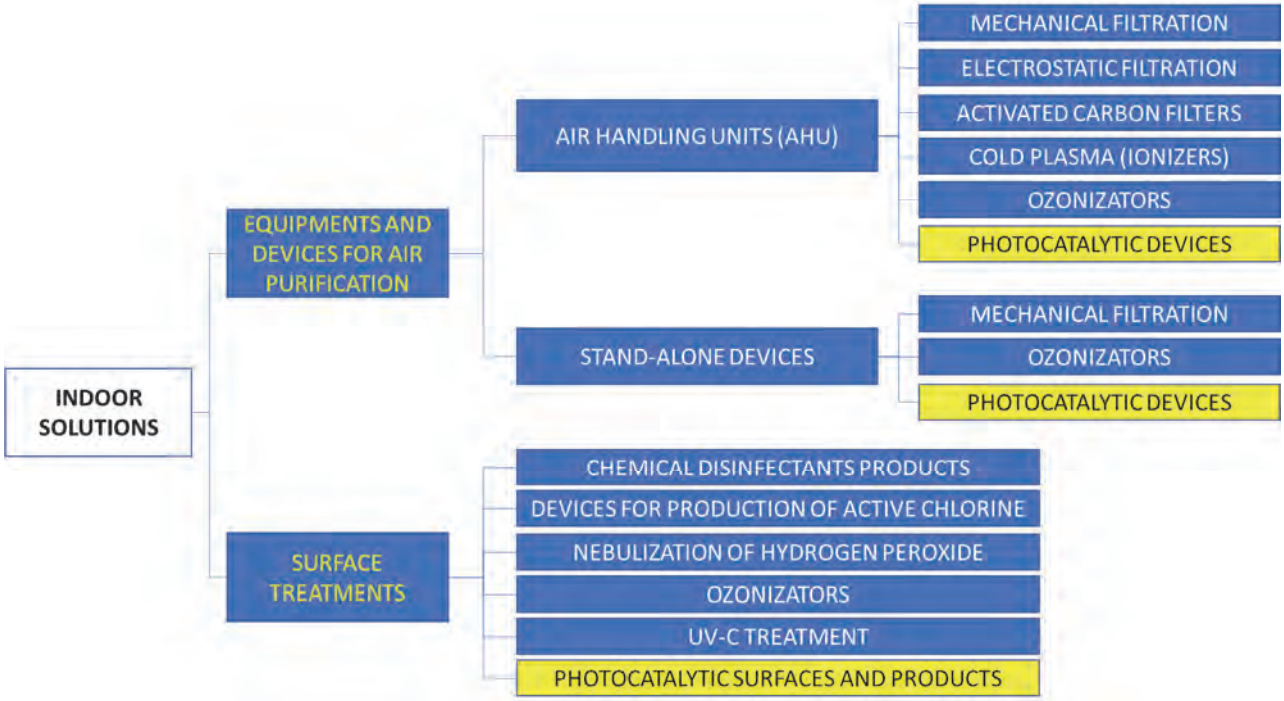
Further, the most promising and innovative solutions both for surface sanitization and for air purification are highlighted, and some commercial products are also described: several solutions can be adopted, depending on the different situations (small and medium-sized or large public and private environments, such as schools, banks, airports, hospitals, shopping malls, industrial and commercial environments, sports centres and gyms).

Indeed, it is a question of distinguishing between an air purification/sanitization and a surface sanitization. The two solutions are not competing, they can be adopted individually according to the environmental situations and the places on which we intend to intervene, but they even complement each other and can be adopted for a complete treatment of air and surfaces.

The technology of photocatalysis will be compared with other solutions currently suggested for the inactivation of viruses, to demonstrate that:

It is a valid, economical and environment friendly solution as an alternative for disinfecting chemicals currently used for surfaces and indoor environments (it is a physical treatment that generates active products in situ);

It is a solution which can be adopted in combination with other techniques (e.g. mechanical filtration and/or electrostatic treatment) for a highly effective air purification.


INDOOR SOLUTIONS
EQUIPMENTS AND DEVICES FOR AIR PURIFICATION
AIR HANDLING UNITS (AHU)
MECHANICAL FILTRATION
ELECTROSTATIC FILTRATION
ACTIVATED CARBON FILTERS
COLD PLASMA (IONIZERS)
OZONIZATORS
PHOTOCATALYTIC DEVICES
STAND-ALONE DEVICES
MECHANICAL FILTRATION
OZONIZATORS
PHOTOCATALYTIC DEVICES
SURFACE TREATMENTS
CHEMICAL DISINFECTANTS PRODUCTS
DEVICES FOR PRODUCTION OF ACTIVE CHLORINE
NEBULIZATION OF HYDROGEN PEROXIDE
OZONIZATORS
UV-C TREATMENT
PHOTOCATALYTIC SURFACES AND PRODUCTS

Access to advanced nanoelectronics and power the IoT infrastructure in Europe

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Abstract:

Development of nanomaterials and their integration into device, from fundamental research to market-ready applications, requires access to advanced tools and expertise that may not be readily available within local networks of academic researchers or companies. Accordingly, the distributed research infrastructure model is particularly suited for supporting and promoting research and innovation in nanotechnology-based products and nanoelectronics. In this talk we introduce two such EU-funded programmes – ASCENT+ and EnABLES, both led by Tyndall National Institute – that offer free-of-charge access to world-leading infrastructure for advances in nanoelectronics and for addressing energy harvesting, storage and management in autonomous devices.

ASCENT+ mobilises an unprecedented network of knowledge and investment, bringing together 15 partners to foster the Nanoelectronics community. ASCENT+ serves as a direct entry point to a European Nanoelectronics Research Infrastructure of global scale offering access to key enabling capabilities in state-of-the-art processing, modelling and simulation data sets, metrology and characterisation, and devices and test structures. Focus areas include:

- Quantum advantage using solid-state platforms
- Low-power, energy-efficient, high-performance computing based on disruptive devices
- Increased functionality through advanced integration of a diverse range of materials and innovative technologies

ASCENT+ offers an unparalleled opportunity to users, empowering them to respond to new problems and to advance knowledge and technology through generating novel results. ASCENT+ enables and stimulates its user community to bridge the gap between scientific exploration and development of proof-of-concept technologies to accelerate innovation pathfinding.

EnABLES integrates key European research infrastructures in powering the Internet of Things (IoT). Six research institutes together with 5 knowledge hubs of excellence address the long-term needs of energy management in self-powered smart sensor systems as required by IoT innovation. Through providing access to unique infrastructure, world-leading expertise, advanced equipment and state-of-the-art technologies, EnABLES empowers hundreds of academic researchers and technologists to advance energy harvesting, storage and micro-power management solutions for the integrated design and deployment of miniaturised autonomous sensors. Nanotechnology offers many opportunities to enhance material/device performance as well as miniaturize ‘power IoT’ solutions. Access ranges from materials & models to devices

and systems and the access providers work with the user community to accelerate adoption and innovation in real-life applications. The EnABLES integration offers a paradigm shift in building an infrastructure network that links new scientific knowledge with application-driven research.

Water and wastewater treatment by heterogeneous photocatalysis: results, process limitations and prospects

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Although heterogeneous photocatalytic processes (HPPs) have been widely investigated in water and wastewater treatment, even with interesting and encouraging results, different obstacles to their application at full scale still exist. In this talk the results from investigations of HPPs will be introduced and discussed with regard to different pollutants and water matrices. In particular, the application of HPPs to drinking water treatment for the oxidation of As(III) to As(V) as well as for surface water disinfection respectively, will be discussed. Moreover, the possible application of HPPs as advanced treatment method of urban wastewater for the removal of contaminants of emerging concern and inactivation of (antibiotic resistant) pathogens, will be also addressed. Industrial wastewater treatment by HPPs will be introduced through examples related to food azo dyes and wastewater containing sugars. In particular, the investigation of agro-food wastewater treatment by HPPs is of interest also in relation to the possibility of energy recovery. For example, hydrogen production during photocatalytic treatment of wastewater containing high concentrations of sugars (particularly glucose) is a potential attractive option for producing energy while removing pollutants from the water matrix. Finally, the limitations of HPPs and possible competition with consolidated or short term perspective technologies for water and wastewater treatment will be discussed.

Bacterial inactivation at the interface of sputtered photocatalytic surfaces without ions release: photo-generated intermediates and possible mechanisms.

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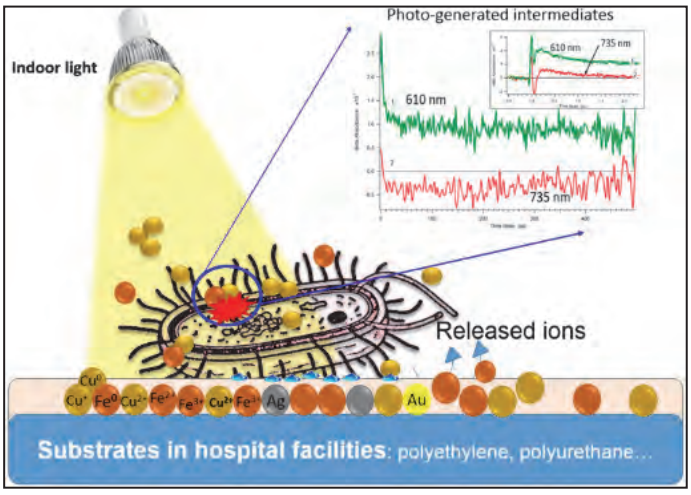
When contaminated with infectious agents, fomites can transfer disease to a new host. In the last years, the role of fomites in disease transfer is higher than ever. Europeans and Americans spend more than 80% of their time indoor [1]. Fomites are associated particularly with hospital-acquired infections (HAIs), as they are possible routes to pass pathogens between patients. It worries epidemiologists and hospital practitioners because of the growing selection of microbes resistant to antibiotics. Today, there is an urgent need for solutions allowing contact microbial adhesion and killing on different fomites' materials.

Catalytic materials/surfaces are attracting a lot of attention during the last decade. However, very few research groups tried to focus on novel materials showing long-lasting catalytic activity killing/inactivating microbes (bacteria, virus, fungi…) [2]. Advanced antibacterial coatings presenting uniform particles distribution, high adhesion to the substrate, mechanical resistance and faster bacterial/biofilm inactivation under light or in the dark are needed due to health concerns. TiO_2 films have been used under light < 387 nm generating highly oxidative radicals as bactericide films for many years. However, its restricted absorption of solar/visible light and slow bacterial inactivation kinetics has motivated researchers to couple TiO_2 with metals (i.e. Cu, Au, Ag or Fe) to shift the light absorption of the films to the visible region [3,4]. In this talk, I will show the coupling of wide bandgap (WBG) semiconductors with narrow bandgap (NBG) metal oxides leading to bacterial/microbial inactivation in the minute range under low intensity indoor light. A brief comparison of the bactericidal activity of NBG bimetal oxides' system compared to WBG will be presented and discussed. Future trends in this field will also be discussed [5].



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Tuning Surface Chemistry of Black Anatase TiO_2 Nanofibers for Photocatalytic Applications

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This work is an appraisal for the photocatalytic degradation of the doxorubicin (DOX), a model antibiotic and a highly toxic chemotherapeutic pharmaceutical employing black titanium dioxide (b-TiO_2) nanofibers as the potential photocatalyst. Here, the surface chemistry was primarily studied to understand the adsorption/desorption kinetics of DOX onto the surface of b-TiO_2. The mode of interaction between DOX and b-TiO_2 was also confirmed *via* Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). In addition to this, we have also investigated the generation of different reactive oxygen species (ROS) including hydroxyl radicals (•OH), singlet oxygen ($^1O_2$), and superoxide anion radical ($•O^{2-}$) responsible for the DOX degradation at the surface of the b-TiO_2 using electron paramagnetic resonance (EPR) spectrophotometer. The obtained data exhibited the formation of $•O^{2-}$ as primary oxidants in the overall reaction. These results were further supported by the alignment of energy levels plotted *vs.* the standard hydrogen electrode (SHE) which also asserted the possibility of $•O^{2-}$ formation as the major reaction intermediate. Finally, the kinetic studies revealed that almost 70% of the DOX was degraded in about < 10 minutes. Compared with the photodegradation of non-adsorbed DOX species in solution (pH 4), the adsorption-dependent surface oxidation (pH 7) by light-induced holes on b-TiO_2 was more efficient, which means that the adsorption of DOX particles is the rate determining step to achieve an efficient degradation. Finally, the liquid phase analysis for the degradation products was also performed by mass spectrometer.

Trace elements Photo-Analysis for environmental applications: a case study

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The origin of rare fragments space rocks fallen on the ground in Ipate area (Iasi County, Romania) following a huge sonic boom felt over a large area of Iasi County was investigated based on the trace elements Photo-Analysis. The material of the samples proved to be insoluble in all the solvents used for tests (water and organic solvents) which makes it be assigned as insoluble organic material (IOM). This, together with the functional groups resulting from the FTIR analysis denoting vibrations similar to those identified on the FTIR spectra of the Murchison, Bells and Allende carbonaceous chondrite meteorite samples raised the question on the nature of the fallen fragments, in correlation with the high intensity sonic boom. Thus, the presence of aromatic and aliphatic compounds, carboxylic acids and / or amino acids, amides, as well as silanol or Si-O groups, carbonates, but also C60 fullerene structures were identified. Water adsorbed on the surface of the material was also identified on the FTIR spectra, as well as adsorbed CO_2. Thorium oxide specific vibrational bands were also observed on FTIR spectra. The investigation on the chemical composition was completed by the analysis of the elemental composition in EDS and LIBS. Analyzing the images acquired with electron microscopy technic (SEM), the morphology and topography of the fragments' surfaces studied in different conditions (bulk and powder) evidenced structures that may be assigned to chondrules and chondrites of carbonaceous meteorites (CM). By mapping the elements identified with EDS on the SEM images, inclusions of calcium and aluminum (CAI), Fe-Ni (Kamacite) and FeS (Troillite), carbonaceous chondrites (CC) with carbon bound to O and S, thorium as ThO_2 were highlighted, as well as finely dispersed or aggregated SiO_2. Crystalline structures were identified in the diffraction patterns obtained by XRD and in the baseline of the FTIR spectra. All the information gathered by these complex analyses and the association with the sonic boom that preceded the fall of the studied fragments provide a number of data and clues that make of interest to further studies on the subject.

Keywords: carbonaceous chondrite, meteorites, LIBS, volatile meteorites, crystallinity

Synthesis of ZnO with enhanced photocatalytic activity using a sacrificial biomass support and Li_2O as doping agent

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Our study was focused on the synthesis of photocatalytic materials for the degradation of organic dyes based on the valorization of biomass resources.

The conversion of biomass into new products with added value can be achieved through different processes such as: combustion, torrefaction, liquefaction, gasification and pyrolysis [1]. According to European Directive 2008/98/EC, pyrolysis is considered a recovery operation and recycling technology [2] that contributed to the obtaining of bio-char from pyrolysis of biomass [3] due to its decontamination potential and disinfection characteristics. In this study, the biochar resulted from pyrolysis process of cherry pits. Activated (by CO_2) flow and inactivated carbon was used to obtain carbon-based photocatalysts impregnated with different zinc salt precursors. The activation of carbon had no significant influence on the photodegradation process. Based on different synthesis procedures, one of our aims was to use an "*in situ*" synthesis method with the advantages of an "*ex situ*" technique [4]. Therefore, our approach involved the use of several zinc salts aqueous solutions to impregnate the biochar structure followed by solvent removal and calcination of the biochar and generation of semiconductor materials in order to investigate the effects on the morphology of the obtained ZnO and its photocatalytic activity. Doping agents like copper, yttrium, silver, cerium, etc. ranging from 1 to 5% in weight were used to decrease the energy band-gap of ZnO or TiO_2 [5] in order to create oxygen vacancies and prevent the recombination of electron-hole ($e^- - h^+$) pairs, thus increasing their photocatalytic activity also in visible light. Until now, few studies demonstrated that the use of Li_2O as dopant may enhance the performance of certain metal oxides like Co_3O_4, Mn_2O_3, CuO, in terms of catalytic activity or sensitivity [6] due to the morphologic modifications that appear during the synthesis process which led to increased specific surface area of the inorganic final materials. Thus, the aim of our study was to investigate the role of biomass carbon as support on one hand, and the role of Li_2O as dopant (using Li_2CO_3 with concentrations as precursor) on the other, for ZnO-based photocatalytic structures for the decomposition of methyl orange. The presence of Li atoms led to photocatalytic activities of the doped ZnO similar to the undoped ZnO obtained at higher concentrations of zinc acetate precursor.

Acknowledgement This work was financially supported by the project Smart polymers obtained by novel photoATRP and 3D printing strategies (SmartPhoto-ATRP), PN-III-P1-1.1-TE-2019-1387 (contract number TE 141/2020), financed by the Executive Unit for Financing Higher Education, Research, Development and Innovation (UEFISCDI).

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Transition metal sulfides-based photocatalytic materials derived from mining and metallurgical wastes

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Over 100 billion tons solid wastes from mining and metallurgical industries are generated annually worldwide. Due to their low intrinsic values and the remote location of most mining operations, over 95% of wastes end up being disposed in landfills, which have an irreversible damage to the environment and constitute a hazard to humans. Therefore, a circular economy model must be formed, which promotes zero waste generation through recycling and re-use of these waste materials and reduces the cost of final products.

In this study, ZnS- and MoS_2-containing wastes from the mining-metallurgy industry were characterized as useful photocatalysts and sensors. Trigonal $ZnIn_2S_4$ layered crystals were synthesized by a binary-flux method using the ZnS-containing waste. Among the binary fluxes used, the KCl:$InCl_3$ was found to be the most favorable for the synthesis of phase-pure trigonal $ZnIn_2S_4$ layered crystals.

The UV-vis diffuse reflectance spectrum exhibited the onset of the absorption edge at approximately 700 nm for trigonal $ZnIn_2S_4$ layered crystals. The presence of secondary crystalline phases (ZnS or In_2S_3) in $ZnIn_2S_4$ layered crystals grown using NaCl:$InCl_3$ and $CaCl_2$:$InCl_3$ fluxes improved the photocatalytic activity, and the photocatalytic H_2 evolution rates reached 188 μmol·h^{-1} and 232 μmol·h^{-1}, respectively, because of efficient separation and transfer of photogenerated charge carriers (Figure 1).

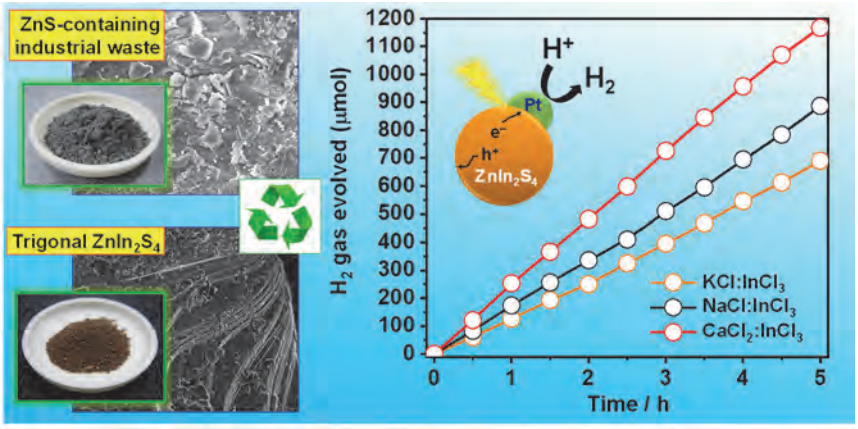

Figure 1. SEM images of ZnS-containing industrial waste and flux-grown $ZnIn_2S_4$ crystals and time courses of H_2 evolution over $ZnIn_2S_4$ crystals grown using different binary fluxes.

The antibacterial activity of ZnS-containing industrial waste against four bacterial strains was studied under UV light irradiation. The antibacterial activity against *L. innocua* was comparable to that against *MRSA*. The inactivation rate against *E. coli* reached 99% within 2 hours of UV light irradiation, while the inactivation of *S. enteretidis* was less effective. Next, we have characterized molybdenite concentrate from the mining-metallurgy industry as a valuable starting material for the fabrication of an efficient and low-cost nanostructured gas sensor. After liquid nitrogen exfoliation, impurities were removed, and the enriched molybdenite-2H was deposited on different substrates by spin coating and drop casting. It was found that spin coating was advantageous over drop casting in fabricating a homogeneous and dense molybdenite-2H film.

The gas sensing behavior of the fabricated sensor was studied for different concentrations of NO_2 at different temperatures. It was found that the temperature strongly influences the key sensing parameters of the device. The sensing behavior of the fabricated device was explained based on the charge-transfer mechanism. The findings of this study reflect a straightforward approach for converting metal sulfide-containing industrial wastes into an efficient photocatalysts and sensors.

Photocatalytic organic synthesis: from nanomaterials to process intensification

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The cost-effective and environmental-sustainable production of pharmaceutical ingredients, agrochemicals, nutrition components, flavors and fragrances gained increasingly importance in the present economy. In general, heterogeneous photocatalysis has been appointed as a promising alternate route for chemical synthesis of base chemicals for those applications. Compared to conventional processes, it has the enormous advantage of operating under mild temperature, exempted of using hazardous reagents and with the prospect of using low energy consumption irradiation sources. Moreover, specific types of reactions can be undertaken at high conversions and yields. The key for the application of such processes lays in the successful combination of effective (photo)catalysts, energy-efficient light sources, and reactor engineering.

Graphite-like carbon nitride (g-C_3N_4) is a polymeric semiconductor which may be regarded as "doped" graphite in which carbon atoms are regularly substituted by nitrogen atoms. The main bottlenecks for the application of this metal-free photocatalyst are the low surface area and the low photonic efficiency. This talk will present several approaches for boosting the activity of g-C_3N_4 for photocatalytic organic synthesis. In addition, the use of such materials in structured photoreactors, seeking for process intensification, will be discussed.

Acknowledgements

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Plasmonic photocatalytic for environmental applications

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Plasmonic photocatalysts, wide-bandgap semiconductors modified with noble metals (NMs) with activity under vis irradiation due to surface plasmon resonance, have been extensively investigated as a possible solution to energy and environmental problems. Although various reports on plasmonic photocatalysts have already been published, the quantum yields of photochemical reactions are usually too low for commercialization [1]. It has been proposed that preparation of plasmonic photocatalysts with efficient light harvesting and inhibition of charge carriers' recombination might result in improvement of photocatalytic activity. Among various strategies, nano-architecture of plasmonic photocatalysts seems to be one of the best methods, including the design of properties for both semiconductor and NMs, as well as the interactions between them [2-3].

Accordingly, our studies have focused on preparation of plasmonic photocatalysts by various approaches, including (i) efficient light harvesting, e.g., polydispersity of NMs (Larger mean size of NM NPs correlates with higher polydispersity in their size and shape.), bi-/tri-metallic photocatalysts, plasmonic photocatalysts co-modified with other absorbing components (ruthenium complexes [4]), and incorporation of NMs inside voids of inverse opal titania structures with slow-photon effect [5], and (ii) fast "hot" electron transfer. Interestingly, it has been found that some highly UV-active titania-based photocatalysts, e.g., NM-modified decahedral anatase particles (DAP) with two kinds of facets ({101} and {001}), show negligible vis activity (Fig. 1), due to unwanted charge carriers' recombination [6]. In contrast, another faceted anatase titania with only one type of facet ({101}–octahedral anatase particles; OAP) exhibits photocatalytic activity one order of magnitude higher, being the most active titania-based particulate photocatalyst (among tested samples), probably due to fast "hot" electron transfer via shallow electron traps [6-8]. The properties, activities (hydrogen evolution, decomposition of organic compounds and microorganisms' inactivation) and mechanisms' clarifications will be discussed during presentation.

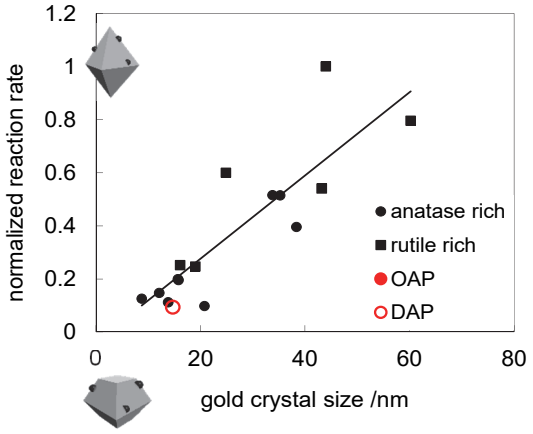

Fig. 1. Comparison of photocatalytic activity of gold-modified titania commercial samples with that by gold-modified faceted anatase titania: OAP and DAP.

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Metal oxide based photocatalysts for environmental applications

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Over the few years, many semiconductor photocatalysts have been explored to degrade the emerging contaminants (e.g. dyes, antibiotics etc.) in the view of environmental protection. So far, TiO_2 and ZnO photocatalysts are commonly used semiconductor materials because of its non-toxic, eco-friendly, low cost and high efficiency. But its use in practical applications limited due to wide band gap and high recombination rate of photo-induced electron-hole pairs. Decoration of noble metals on the semiconductors (TiO2 and ZnO) helps to solve these problems by surface plasmon resonance (SPR), which helps in enhancement in visible light absorption and hinders electron-hole pair recombination. In this talk, I will show the decoration of Ag on semiconductor materials (TiO_2 and ZnO), study the structural/morphological features and enhanced photodegradation performance on emerging contaminants. Effect of noble metal concentration, SPR effect and plausible photocatalytic mechanism will be discussed.

Keywords: Metal Oxides; Photocatalysis; Dyes; Antibiotics;

Computational materials design of halide double perovskites: Possible novel visible-light photo-catalysts

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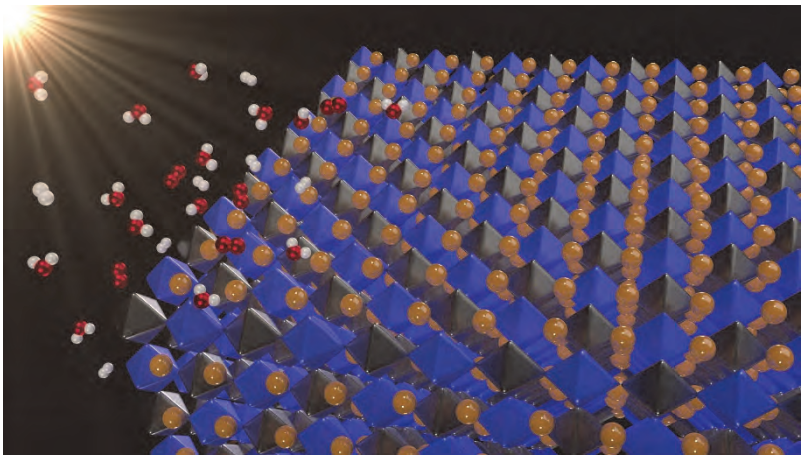
Lead-based halide perovskites have emerged as the most prominent candidates for emerging photovoltaic technologies. In this talk I will briefly showcase recent efforts towards designing new Pb-free semiconductors that are alternatives to traditional halide perovskites, for which computational approaches from first-principles have been extensively successful and revealed a series of new compounds within the so-called halide double perovskites family and vacancy ordered perovskites. Among these, $Cs_2BiAgBr_6$ has the narrower indirect band gap of 1.9 eV, [1] and $Cs_2InAgCl_6$ is the only direct band gap semiconductor, yet with a large gap of 3.3 eV. [2] All of them exhibit low carrier effective masses and consequently, are prominent candidates for a range of opto-electronic applications such as photovoltaics, light-emitting devices, sensors, and photo-catalysts. [3-4] I will specifically outline the computational design strategy that led to the synthesis of these compounds, and particularly focus on the insights we can get from first-principles calculations in order to facilitate the synthesis, improve their opto-electronic properties and the in-silico identification of compounds with properties that are similar to the lead-halide perovskites.



Within this talk, I will also showcase the power of calculations from first-principles to investigate the surface and interface properties of the newly designed compounds, and show how in fact $Cs_2BiAgBr_6$ and $Cs_2BiAgBr_6$ are in for photocatalytic water splitting. The newly developed concept of analogs led us to identify a new oxide double perovskite semiconductor, Ba_2AgIO_6, which exhibits an electronic band structure remarkably similar to that of our recently discovered halide double perovskite $Cs_2AgInCl_6$, but with a band gap in the visible range at 1.9 eV. [5] In the last part, I will employ this strategy to explore the phase space of

vacancy-ordered double perovskite and discuss the case of Zr-based compounds as alternates to Cs2TiX4 with X=Br,I. [6]

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Theoretical investigation of low-dimensional materials for photocatalysis

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Recent interest in photocatalysis is related to environmental concerns and to the search for viable methods for clean energy production and storage. Replacement of fossil fuels by sustainable energy resources may become possible by harnessing solar energy, provided efficient and cost-effective technologies are available for collecting, converting and storing this energy. Research activity to overcome these challenges is intense and focuses on the development of innovative materials and processes. Despite enormous progress in sunlight harvesting, photovoltaics (PVs) with combinations of band gaps designed to absorb within a large portion of solar radiation's spectrum is an active field of research. The greatest challenge though is the storage of intermittent solar energy. An attractive option is to produce hydrogen, a good energy carrier, from electrolysis of water using electricity provided by PVs. Then, hydrogen and oxygen can be used in fuel cells to produce electricity and water. The best available catalysts are platinum-based materials and research in electrochemistry on inexpensive alternatives is ongoing. Photoelectrocatalysis, i.e., combining photovoltaics and electrolysis, requires considerable effort in designing stable, efficient, and inexpensive materials and devices. Molybdenum disulfide (MoS_2) and other semiconducting transition metal dichalcogenides (TMDs) are promising materials for applications in optoelectronics and catalysis. Over the last few years, 2D and quasi-1D TMDs have attracted a lot of attention. We have studied theoretically TMDs, other emerging low-dimensional materials, and their heterostructures. TMD band gaps, which are in the visible range and become direct in atomically thin monolayers, as well as other electronic and dielectric properties, can be modified with dimensionality, strain, substrate, nanostructuring, etc. [1-4]. Focusing on the hydrogen evolution reaction (HER), we will present theoretical results based on density functional theory, which show that besides its active metallic edges [5], the otherwise inactive MoS_2 basal plane becomes active by defects and transition metal doping [6]. We will discuss the potential of TMDs as cocatalysts in HER and environmental remediation together with some recent examples.

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PVDF fibers embedding lanthanide doped ZnO membranes for adsorption and photocatalytic degradation of dye organic pollutants

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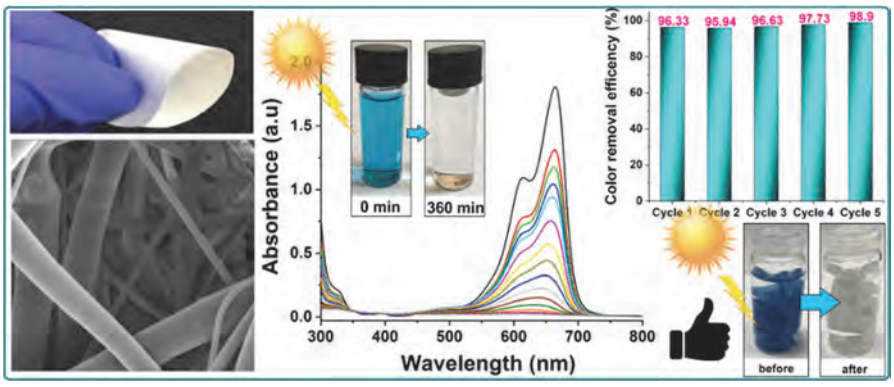
New hybrid materials based on lanthanide doped ZnO nanoparticles (Ln=Sm,La,Er) [1,2] reinforced in PVDF membranes were prepared by electrospinning method, materials that have not been reported so far. The materials were evaluated in terms of crystalline structure (XRD), surface morphology (SEM), mechanical and adsorption/desorption properties. SEM measurements highlighted a continuous, uniform, and bead-less formation in the optimal electrospun conditions morphology. The results from the mechanical evaluation showed that PVDF/ZnO:Ln nanostructures had higher values of the elongation at break as compared to pristine PVDF. As the ZnO:lanthanide level increased, the elongation at break increased too. Thus, the elongation at break for pristine was 45.49 MPa, and for the materials containing 37 % ZnO:lanthanide was up to 71.09 MPa. The photocatalytic activity towards MB (10 mg/L) and RhB (5 mg/L) degradation under visible light irradiation was performed for all prepared materials. The excellent color removal efficiency was up to 96.33 % for MB and 93.36 % for RhB removal for the membrane containing 37 % ZnO:La. The results were validated by the photodegradation kinetics evaluation which followed a pseudo-first-order kinetic model. The calculated values of the rate constants were between 10^{-3} to 10^{-2} min^{-1}, depending on the percentage of ZnO:lanthanide and initial dye concentration. Moreover, the materials could be recovered and reused even after five repeating cycles with the photocatalytic activity up to 98 %. In addition, it can be pointed out that the degradation process takes place in the environment-friendly conditions (under visible light irradiation), promoting this way the applicative potential of the present PVDF/ZnO:Ln membranes in industrial dye wastewater treatment.



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Halide Perovskites: The Emergence of a New Class of High-Performance Semiconductors

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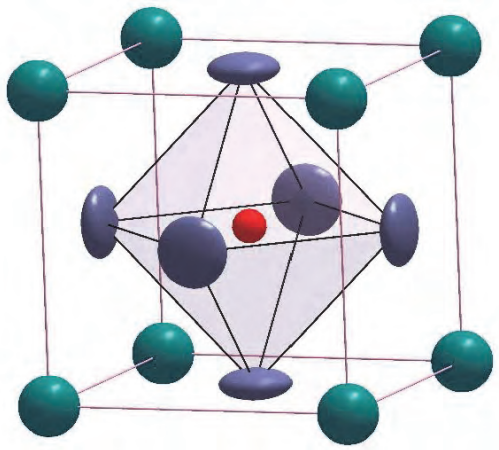
Halide perovskites is the new edition of the namesake family of materials that has revolutionized science, from the discovery of high-performance ferroelectrics ($BaTiO_3$) and high-Tc superconductors ($YBa_2Cu_3O_7$) for over a century *(1)*. The most recent iteration of perovskites -the emerging class of halide perovskites- is a family of high-performance semiconductors which operate in the visible and infrared energy range. These materials, known for over a century, were suddenly brought back to life in the 1990's with the pioneering work of D.Mitzi *(2)* and G. Papavasiliou *(3)*, but the genuine breakthrough came in 2009, when T. Miyasaka and co-workers demonstrated that the hybrid organic inorganic perovskite, $CH_3NH_3PbI_3$, can be employed in photovoltaics *(4)*. What followed since this original discovery was a resurgence of interest for these materials resulting in a highly competitive research race towards solution-processable, cost-efficient and high-performance solar cells. To date this race is still raging, reaching record power conversion efficiency of ~25%, pending commercialization. Along the rapid development of solar cell technologies, it also became apparent that halide perovskites possess altogether remarkable semiconducting properties applicable to all field of optoelectronics. These remarkable physical properties derive from



their unique electronic structure, which lends the semiconductors high absorption coefficients and charge-carrier mobilities.

Figure 1. The crystal structure of the ideal cubic from of the perovskite family.

In this presentation I will outline the compositional space of the halide perovskites, AMX_3, (A^+ = Cs, CH_3NH_3, $HC(NH_2)_2$); (M^{2+} = Ge, Sn, Pb); (X^- = Cl, Br, I) and explain the crystal chemistry of the materials, as well as their low-dimensional and compositional derivatives. I will discuss how small changes in the crystal structure can significantly alter the optical, electrical and electronic properties of the perovskites and I describe how these can be controlled by targeted chemical synthesis. Lastly, a brief synopsis of how halide perovskites can be applied in

optoelectronic devices, tackling device-specific problems such as environmental instability and toxicity will be presented

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2D/2D Heterojunction Photocatalysts for Sustainable Energy and Environmental Applications

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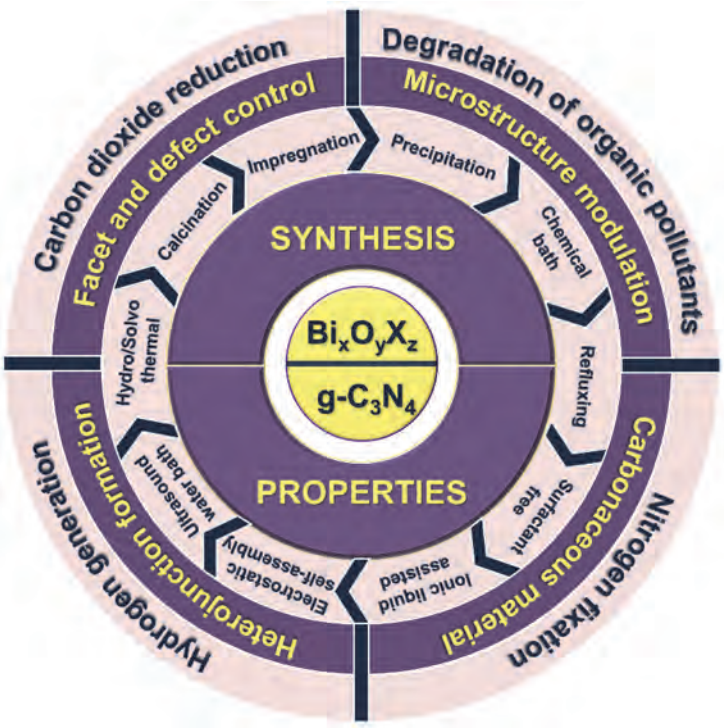

Recently, the construction heterojunction photocatalysts, especially 2D/2D systems with two dissimilar layered semiconductors in face-to-face contact has drawn immense attention due to their synergistic influence. 2D layered structures of Bi-rich $Bi_xO_yX_z$ are active semiconductor photocatalysts with higher photon absorption efficiency, which induces greater electric field intensity and subsequently leads to large dipole moment. The larger dipole moment and wider interlayer spacing in $Bi_xO_yX_z$ boosted by the large polarization force and polarization space lead to increased internal electric field, which in turn enhances the separation efficiency of the photogenerated charge carriers. Also, as suggested by recent studies sandwiching 2D layered semiconductors of BiOX/$Bi_xO_yX_z$ and g-C_3N_4 conveniently promotes the formation of a heterojunction that can facilitate enhanced photocatalytic performance aided by their favorable band positions. In this talk, I shall be summarizing some of the recent advances of BiOX/$Bi_xO_yX_z$-g-C_3N_4 heterojunction photocatalysts for selective applications. Also, the perspectives and plausible opportunities in the development of high performance BiOX/$Bi_xO_yX_z$-g-C_3N_4 heterojunction photocatalysts shall be discussed.

Atomistic modeling in Photocatalysis

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Photo and photoelectrochemical processes require the fine tuning of the properties of the adsorbers and the materials acting as catalysts. In the present talk I will revise some of the latest developments in our group that demonstrate the need to understand how interfaces work and the challenges ahead in this type of modeling.

Antibacterial Textiles Using Visible Light Using Manganese Doped TiO_2 Nanoparticles

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Moisture, different contaminants and sweat that constitute their micro-climate, favour microbial and bacterial growth in textiles, while in use. Hence, textiles can easily become malodorous and the source of cross-infections. It is then evident that following hygiene, but also comfort, requirements, that functionalization of textiles in order to gain antibacterial activity, as well as self-cleaning properties are of paramount importance. To this end, simple approaches of surfaces modification using different functional materials have been widely used.

Here, we present a simple and low-cost technique to prepare antibacterial, photocatalytic and self-cleaning cotton textile fabrics. The fabrics were functionalized by spray coating with manganese (Mn)-doped photocatalytic titanium dioxide (TiO_2) nanoparticles, using polydimethylsiloxane (PDMS) as binder. The TiO_2:Mn nanoparticles were prepared by a sol gel method, followed by mill balling to achieve an average diameter of approximately 100 nm.

Different TiO_2:Mn and PDMS ratios were used, and subsequently, the treated fabrics were characterised for their chemical and physical properties. The functionalisation did not result in alteration of the mechanical properties of the textiles, in particular the mechanical properties worsened less than 20% and porosity was found to be similar to the untreated fabrics. Furthermore, the functionalized fabrics were characterized for their anti-bacterial properties against both against *S. aureus* (Gram-positive) and *K. pneumoniae* (Gram-negative) bacteria, and displayed 100% reduction of both kinds of bacteria within 120 min under natural sunlight. Finally, the treated fabrics demonstrated complete photocatalytic degradation of methylene blue (MB) dye adsorbed on their surface under both UV and visible irradiation, turning them white.

In addition, the modified fabrics were also resistant to several laundry cycles. Physical properties like mechanical strength, colour, breathability and aesthetic of the prepared cotton fabrics remained unchanged. The presented modified cotton fabrics can be envisioned as antibacterial, anti-odorous and self-cleaning textiles for sports, medical uses, uniforms, fashion, home furnishing and leisure activities.

Co-creation of future cities - EFdeN Sustainable City

Csatlos, Ioana – Sustainable Development Manager & Vicepresident Solar Decatlon Bucharest Association, EFdeN

EFdeN is one of the most well-known student NGOs in Romania that works in the field of sustainability. We are a multidisciplinary team of over 60 students and recent graduates of various specializations, passionate about sustainability and change.

Our projects provide volunteering students with a great opportunity for practical and accelerated professional and personal development. We address 5 different public segments: students, children and teenagers, companies and the general public. We host events, workshops and develop educational programs in a **non-formal environment.**

We develop projects and people who want to recreate Romania and the cities in which they would like to live. We focus on sustainability and climate change, youth and the environment.

In all activities we follow the development directions proposed by the UN for 2030, adhering to the Sustainable Development Goals.

A sustainable city starts with small steps.

EFdeN Sustainable City project will allow visitors to experiment what it would be like to inhabit a city like this, aiming to transform the cities we live in for the next generations.

We are showcasing elements of a smart and sustainable city and the way they work together, by representing 8 of these main components through practical projects and themed areas, testing them and communicating the results.

The 2 houses EFdeN has developed in the past 6 years are placed next to each other, working as a combined research center for new projects.

We have to accelerate the transition towards a clean energy economy. At EFdeN we have 2 solar houses that are 100% electrical, 2 solar trees and 2 charging stations for electrical vehicles that will work on a smart grid changing energy between them. All of these in a green campus where students and professionals can work outdoors, with free energy and wi-fi.

We encourage smart mobility with the use of bicycles and electrical scooters, which is why we will integrate renting and charging stations for them. In order to lower our CO2 footprint as much as possible, we have also developed a self-sustainable solar charging station for electrical vehicles.

We encourage reducing your generated waste, using recycled materials and selective collection.

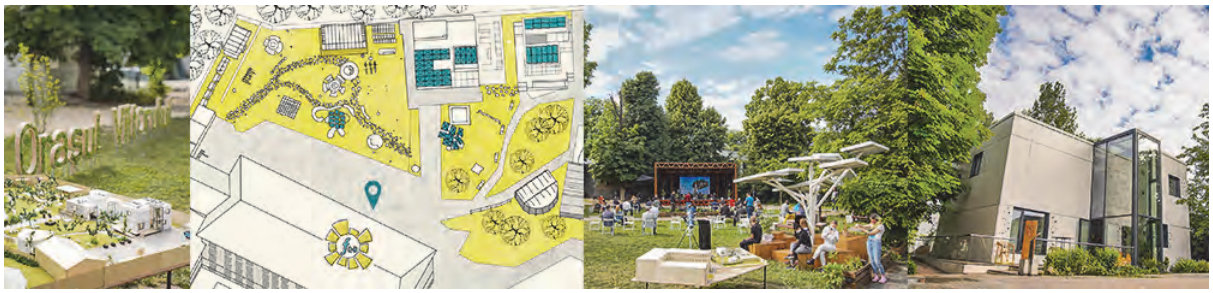
Therefore, we want to integrate recycling and composting stations to divert as much landfill waste as possible.

Both EFdeN houses were designed to integrate the urban farming concept. Both inside the houses as well as around them we support domestic harvest of productive plants in the urban area, as a healthy and economical alternative for the inhabitants.

We spend 80% of our time inside buildings and this affects our health and productivity. The Sick Building Syndrome is one of the subjects we have approached in developing The Guide of Comfort Conditions.

We want to extend our activity range, in the field of Health & Well-being, with guides, events and activities in sports and nutrition.

And last but not least, innovation for a circular city.



ORAL PRESENTATIONS

2D/2D Ni-doped MoS_2/g-C_3N_4 Layered Hetero-Nanostructures as Highly Efficient Photocatalysts for Environmental Remediation

Eirini D. Koutsouroubi[a], Ioannis Vamvasakis[a], Maria G. Minotaki[a], Ioannis T. Papadas[b], Stelios A. Choulis[b], Georgios Kopidakis[a], Gerasimos S. Armatas[a,*]

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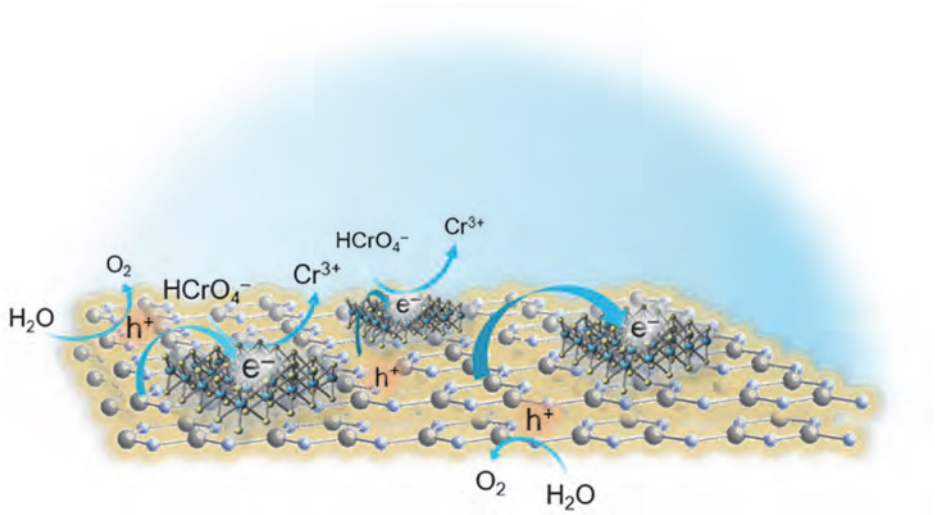
Highly efficient and cost-effective photocatalysts are among the most prominent targets in the field of environmental remediation and clean energy production. Water pollution is on top of the most permeative threats worldwide, risking human health and quality life. This is because voluminous amounts of toxic metals, such as hexavalent chromium, Cr(VI), are released directly or incidentally to the environment. [1] Various photocatalysts have been investigated for the disinfection of wastewaters, but most of them do not exhibit good efficiency and/or chemical stability. Herein, we report that 2D/2D layer heterostructures composed of exfoliated Ni-doped MoS_2 nanosheets and graphitic carbon nitrite (g-C_3N_4) layers can carry out photocatalytic Cr(VI) reduction in aqueous solutions with outstanding activity, reaching apparent quantum yields up to 29.6% at 375 nm and 23.7% at 410 nm, which are the highest among all reported nonprecious catalysts. [2] We show that doping the MoS_2 lattice with Ni markedly increases the photochemical activity, which, together with electrochemical, spectroscopic and theoretical DFT computational studies, arises from the enhanced charge carrier density and mobility at the interface of Ni-doped MoS_2/g-C_3N_4 junctions. In addition to the favorable charge transport properties, delineation of the photoinduced oxidation reactions by gas monitoring techniques reveals that the high efficiency in this catalytic system also arises from fast water oxidation kinetics. Due to the efficient dissociation of charge carriers, surface-reaching holes effectively oxidize water to form molecular oxygen. The results of this work mark an important step forward in understanding and designing low-cost and earth-abundant catalysts for detoxification of Cr(VI)-contaminated industrial effluents.



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[3] The authors acknowledge support from the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the "1st Call for H.F.R.I. Research Projects to support Faculty Members & Researchers and the Procurement of High-cost research equipment grant" (Project Number: 400).

Bio-chemo sequential synthesis of silver oxide nanoparticles embedded in TiO_2 shell ($BioAg_2O@TiO_2$): A visible light active photocatalyst

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A sequential bio-chemo synthesis approach has been adopted in the present study to synthesize silver oxide nanoparticles embedded in TiO_2 shell. Ag_2O nanoparticles were synthesized through a bio based method where $AgNO_3$ precursor was reduced using cell free supernatant of a bacteria, *Alcaligens* sp. Further, the biosynthesised silver oxide nanoparticles were embedded in TiO_2 ($BioAg_2O@TiO_2$) through a chemical method involving the hydrolysis of Titanium (IV)-(triethanolaminato) isopropoxide solution (TTEAIP), with Ag to Ti molar ratio of 1:1.7 in the synthesis mixture. The formation of TiO_2 shell embedded with Ag_2O particles was confirmed through X Ray Diffraction (XRD) and Transmission Electron Microscopic (TEM) analysis. The value of apparent band gap energy of $BioAg_2O@TiO_2$ was found to be is 2 eV , indicating its visible light activity. The average crystallite size as determined by Debye Scherrer's formula was 27.1 nm for Ag_2O and 53 nm for TiO_2. $BioAg_2O@TiO_2$ was found to catalyse the degradation of Reactive blue 220 (RB-220) dye under visible light irradiation,confirming it to be a visible light active photocatalyst. The photocatalytic degradation was favored at acidic pH 3. The sequential bio-chemo synthesis approach is novel and a greener approach as compared to completely a chemical method of synthesis.

Foam-like PMMA Microcapsules modified by ALD metal-oxide as photocatalytic materials

Marta A. Forte[1], Ricardo M. Silva[2], Carlos J. Tavares[1], Rui F. Silva[2]
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The development of materials that can efficiently remove persistent and toxic organic compounds from the water is of upmost importance in environmental applications. To this end, photocatalytic materials are an interesting and promising solution because they can use the solar light to activate the photodegradation processes. The semiconductor-based photocatalysts have been applied to wastewater treatment. For instance, metal-oxides are wide band-gap energy material in the near-UV spectral region with a great photocatalytic activity which can be combined with a second material as a support matrix, in order to improve the photocatalytic active surface. Therefore, the preparation of hybrid materials, comprised of an inorganic part and an organic counterpart (polymeric materials) is crucial. Among the different types of polymers, poly(methyl methacrylate) (PMMA) is frequently used in many applications mainly due to its mechanical properties, chemical stability and transparency to visible light. On the other hand, atomic layer deposition (ALD) emerges as a powerful and viable deposition method as it allows for the deposition of metal-oxide crystalline phases at low temperatures compatible with the thermal fragility of PMMA.

Herein, we present a solvent evaporation technique strategy to obtain foam-like PMMA microcapsules due to the slow methylene chloride evaporation. This open porosity geometry is suitable to be coated with metal-oxide ALD allowing the increasing of the photocatalytic active area as well of the physical contact with the wastewater. Therefore, it is expected that the photocatalytic efficiency of this hybrid material will be enhanced, when compared with the individual components. The photocatalytic activity was evaluated by monitoring the degradation of methylene blue as a representative dye pollutant under UV irradiation. Figure 1 reports a schematic illustration of the materials presented in this work.

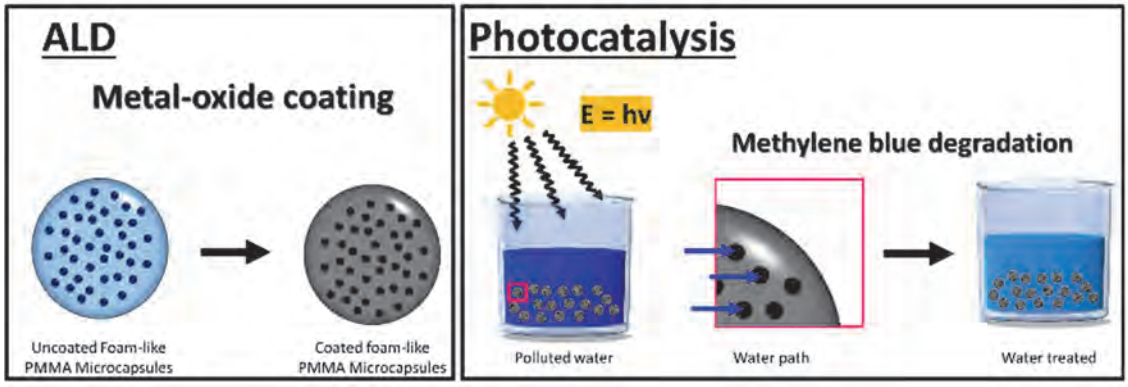

Figure 1. Schematic illustration of the materials preparation.

Gadolinium ortho-ferrite interfaced polyaniline: Bi-functional catalyst for electrochemical detection and photocatalytic degradation of acetaminophen

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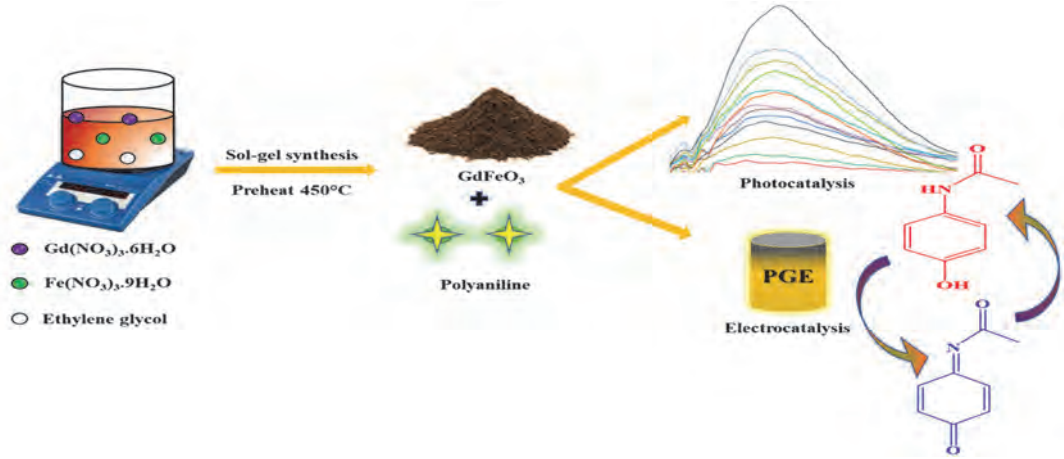
Rare-earth based perovskite in combination with conducting polymers have been time tested and proven effective because of their improved electro-optical and catalytic properties. In the present work, we have synthesized GdFeO3 by glycol assisted sol-gel process and incorporated it into the conducting polymer polyaniline (PANI) to prepare GdFeO3 interfaced PANI nanocomposite (GdFeO3@PANI). The physical and chemical properties of the GdFeO3@PANI were investigated using various spectroscopic and analytical techniques such as XRD, FT-IR, FESEM, EDX and TEM.

Further, the GdFeO3@PANI nanocomposite was employed as bifunctional catalyst for the electrochemical sensing and photocatalytic degradation of analgesics and antipyretic drug acetaminophen. For developing acetaminophen sensor, bare pencil graphite (PE) was modified with GdFeO3@PANI composite and the resulting PE/GdFeO3@PANI sensor was later used in electroanalysis through techniques such as cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The investigations showed that the integration of GdFeO3 into PANI matrix boosted the electron transfer rate making it an excellent electrocatalyst for acetaminophen sensing featuring low peak potential and enhanced cathodic peak current. The analytical performance of the PE/GdFeO3@PANI sensor exhibited wide linear response range, low limit of detection with satisfactory stability, repeatability and reproducibility.



The results of real sample analysis projected a good recovery rate promising the PE/GdFeO3@PANI sensor capable enough to be effectively employed for the quantification and detection of acetaminophen. Apart from examining the sensing properties of GdFeO3@PANI nanocomposite, its photocatalytic behavior in removing acetaminophen from water was also investigated and the composite was found to show excellent photodegradation capabilities whose efficiency is attributed to the enhanced charge separation and rapid electron mobility within the system.

The photodegradation was carried using LED source that makes the system economical and eco-friendly. Hence, the as-prepared GdFeO3@PANI nanocomposite was proved to act as an efficient bi-functional catalyst which could be scaled up for real time detection and remediation of acetaminophen.

H_2 evolution over Cu-impregnated P25-TiO_2 via alcohol photoreforming: an insight on Cu active species

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As a green energy carrier, hydrogen can be produced via sustainable processes employing unlimited energy sources, such as sunlight irradiation. Organic photoreforming is a promising strategy for a clean solar H_2 production that can effectively replace established production processes based on fossil fuels and severe operating conditions. Nanocrystalline TiO_2 (Degussa P25) is one of the most effective photocatalysts. It exhibits a high likelihood of photogenerated charge carrier recombination, although it works under near-UV irradiation.

The addition of Cu species is an effective strategy to enhance P25 photoefficiency due to the formation of a metal-semiconductor heterojunction spatially separating free charges. Although several studies investigated the effect of Cu loading on P25 nanoparticles, the role of Cu oxidation state on the improvement in photocatalytic H_2 generation has not yet been entirely elucidated. Conflicting conclusions in the literature review ascribed the improved photocatalytic activity of Cu/P25 systems to the presence on the TiO_2 surface of finely dispersed and easily reducible CuO_x.

The present study aims at clarifying the nature of Cu species in Cu/TiO_2 photocatalysts preparing samples at different Cu loading via the impregnation-calcination method. Moreover, the evolution of Cu species under UV-Vis irradiation was investigated to identify the active species uniquely. H_2 production rates were integrated with a detailed physicochemical characterization of the catalysts before and after the photocatalytic process through a combined approach of complementary techniques, including X-Ray Photoelectron Spectroscopy, High-Resolution Transmission Electron Microscopy, and Temperature Programmed Reduction analysis. CuO and Cu_2O nanostructures were obtained on the P25 surface by impregnation and further heat treatment. The sample exhibiting the highest H_2 production showed a more significant fraction of finely dispersed CuO nanostructures.

During the process, CuO_x species undergo an in situ dynamic nanostructuring, leading to a considerable change in oxidation state and size distribution. This evolution is related to the dissolution of CuO_x species, followed by reducing Cu^{2+} to Cu^{1+} and Cu^0 by photogenerated electrons. Both Cu_2O and Cu^0 acted as co-catalysts for H_2 generation, as reported in Figure 1.

The obtained findings outline that Cu/P25 photocatalysts are complex and dynamic systems. Their evolution during photocatalytic processes is influenced by solution properties and catalyst preparation methods, which significantly affects the size distribution and dispersion of

Cu species. It ultimately leads to different ratios between Cu oxidation states on the catalyst surface.

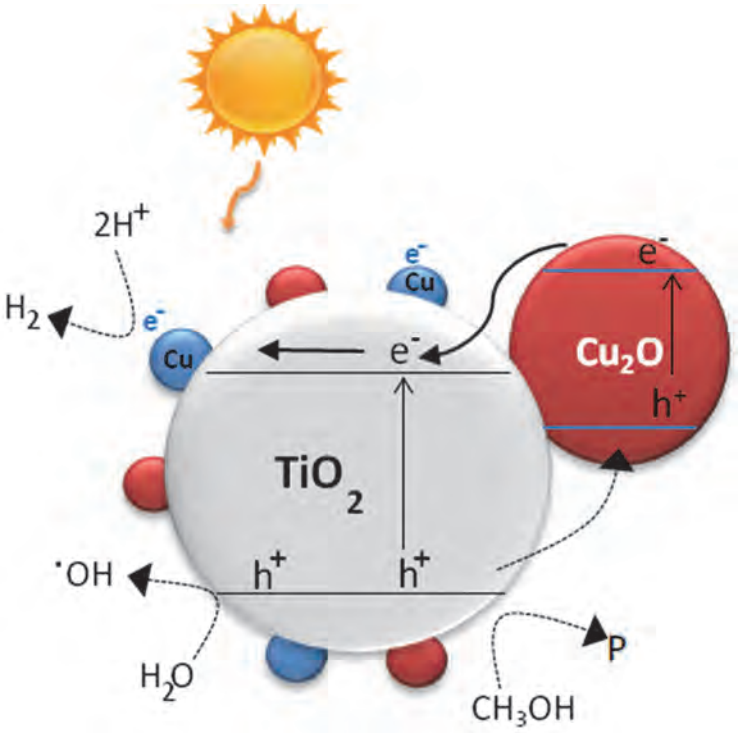

Figure 1. Proposed hydrogen photogeneration mechanism for Cu/Cu2O/ TiO2 system.

Iron-doped cerium oxide/graphene oxide nanocomposites for the degradation of organic pollutants from wastewater

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Rapid development and industrialization have significantly contributed to the pollution of water by toxic substances such as dyes that subsequently run-off into water systems. Unlike other methods, photocatalysis has thus far been reported as a promising solution towards the removal of these toxic species. Cerium oxide (CeO_2) is a rare earth metal oxide with a band-gap of 3.2 eV and has been considered as one of the most promising photocatalysts owing to its high activity and high oxygen transport capacity. However, its larger band-gap limits its application in the UV radiation range. Doping CeO_2 with transition metal ions such iron (Fe) has been reported to reduce the bandgap since Fe can easily substitute for Ce-ions in the crystal lattice of CeO_2. In this work, the proposed Fe-CeO_2 nanoparticles were further combined with graphene oxide (GO) to yield Fe-CeO_2/GO nanocomposites. GO was synthesized using the modified Hummers method and later was as a support for Fe-doped nanoparticles which helped limits the chances of leaching consequently increasing its photoactivity. Fe-doped cerium nanoparticles and Fe-CeO_2/GO were synthesized using a facile co-precipitation method and hydrothermal method, respectively and further characterized using techniques such as XRD, FTIR, PL, UV/Vis, and Raman spectroscopy, among others. The results confirmed formation of the expected nanocomposites. The photocatalysts were further used to degrade unwanted organic pollutants including undesirable acid violet dye in aqueous solutions and high removal efficiencies were achieved.

Laser induced chitin deacetylation- cutting-edge technology for "natural biological waste”

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A new method, Laser Induced Chitin Deacetylation (LICD), to produce chitosan thin films from oyster shell is reported with this work. This new method addresses the concern on the issue of the accumulation of "natural biological waste”, providing new use based on the cutting-edge technology of laser ablation and deposition. The method, consisting in oyster shell irradiation with high power pulsed laser is presented, including parameters and procedures. FTIR spectra of oyster shell and of the obtained thin film validate the method evidencing chitin deacetylation into chitosan based on the physico – chemical processes of laser induced deacetylation. UV-Vis and LIF spectra together with the compared elemental composition analyzed with SEM-EDS technic complete the validation of the results. AFM analysis offers information on the thin film morphology. COMSOL simulation anticipates and confirms the experimental results, also providing information about the conditions required for the physico-chemical processes involved. The LICD method has the potential to be applied both in the experimental field and for the production of medical devices such as transdermal patches with hemostatic and antibacterial effects, food packaging, micro-filters for water decontamination, electronics and optoelectronics components – including solar cells, sensors, as well as in other fields where the thin films of chitosan are of interest.

Keywords: laser induced chitin deacetylation, laser induced hydrolysis, chitosan, composite, medical patches

New La doped TiO_2 nanofibers for photocatalytic degradation of organic pollutants: Effect of thermal treatment and La-doping amount

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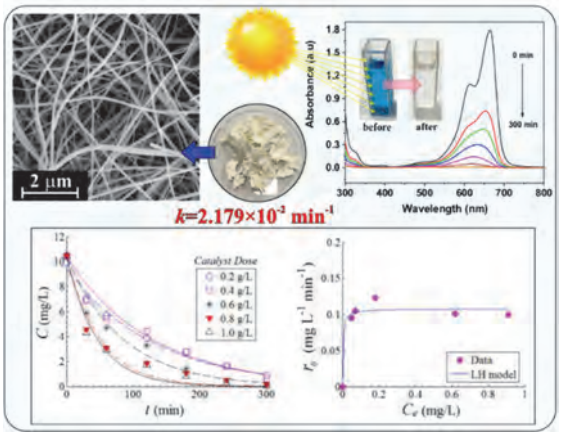
Many studies are based on the development of new oxide semiconductor materials with improved photocatalytic properties for both wastewater treatment and air decontamination under UV or sunlight irradiation. Titanium dioxide (TiO_2) is among the most important semiconductors used in photocatalytic processes due to its remarkable properties such as non-toxicity, low cost, good chemical stability, and high photocatalytic efficiency. Generally, to improve the photocatalytic properties of TiO_2, the most common method is doping this semiconductor material with different metals such as Ag, Cu, Er, Nd, Eu, etc.

We report herein, La doped TiO_2 nanofibrous photocatalysts of various formulations obtained by electrospinning method. The typical characterization of photocatalysts was performed using the X-ray diffraction (XRD), scanning electron microscopy (SEM) and UV–vis spectroscopy. The maximum color removal efficiency found for the degradation of Methylene Blue dye was 99.52 % for an initial concentration of 10 mg/L after 300 minutes of visible light irradiation.

We found outstanding performances for TiO_2 doped with La (0.1%) (calcined at 600 °C) that yielded a maximum value for the constant rate (7.625×10^{-3} min^{-1}). Moreover, at catalyst dosages of 0.2 to 1 g/L, the reaction rate constant attained the order of 10^{-2} min^{-1} under visible irradiation. In addition, the best catalyst sample TiO_2:La(0.1%) was tested in the photodegradation of ciprofloxacin drug (micropollutant) under visible light. Results revealed that after 300 min irradiation time, the photodegradation of ciprofloxacin was found to be 99.5%, whereas the reaction rate constant was equal to 1.981×10^{-2} min^{-1}.



Acknowledgment: This work was supported by a grant of the Romanian Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-TE-2019-0594, within PNCDI III.

Photocatalytic Composite Thin Films with Controlled Optical Properties Based on TiO_2, WO_3 and rGO

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Abstract

The work investigates the self-cleaning and optical properties of composite thin films based on titanium dioxide (TiO_2), tungsten oxide (WO_3) and reduced graphene oxide (rGO) sprayed from dispersions of sol-gel powders. The samples in the first set (Route 1) are obtained through layer-by-layer deposition of TiO_2-rGO and WO_3-rGO coatings, varying their order in the composite. The second set (Route 2) contains one-batch deposited films from a mixed TiO_2-WO_3-rGO powder. Coatings are uniform and continuous, with several aggregates at the surface. All films are photocatalytically-active under simulated solar radiation (34 W/m^2) in phenol and methylene blue (MB) removal from low concentrated solutions. Higher photocatalytic efficiencies recorded for MB removal may be the result of dye sensitization. The improved adsorption of both pollutants on the one-batch films is directly correlated with their improved wetting properties (water contact angle of 11-12^o).

Transmittance higher than 80% and reflectance lower than 15% in the UV-VIS region for all films recommends them for deposition on glazing, with little light penetration hindrance. The slightly rougher samples (Route 1) induce surface light scattering increasing the reflectance.

The stability of the films is evaluated through morphological characterization before and after photocatalysis and shows that the smaller, less adherent aggregates are transferred from the film to the pollutant solution, increasing the thin films surface roughness.

Overall, the Route 2 (one-batch deposition) samples are better suited as self-cleaning layers on glazing compared to the Route 1 thin films (layer-by-layer deposition), as they meet the requirements for self-cleaning coatings and are slightly more stable during the photocatalytic process.

Photocatalytic degradation of toxic phenolic compound and bacterial inactivation by novel Li doped $Zn_{0.5}Ni_{0.5}Fe_2O_4$

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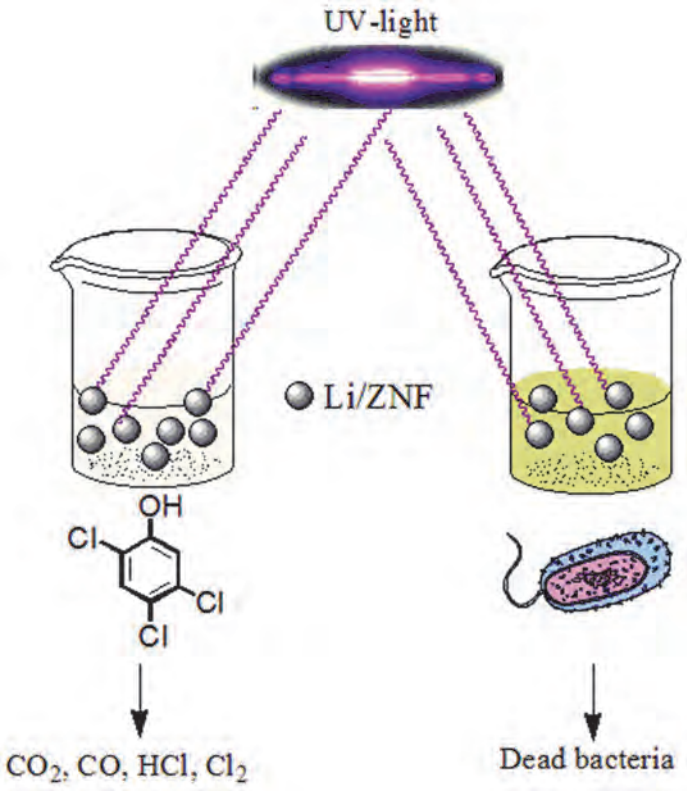
Photocatalysis is a promising cost-effective water treatment and antimicrobial decontamination technology. Here, a novel phototocalyst (Li/ZNF) was prepared for the first time and characterized. Specifically, Li metal was coupled with $Zn_{0.5}Ni_{0.5}Fe_2O_4$ which resulted in a localized surface plasmon resonance and improved the photocatalyst efficiency. Li/ZNF possesses a bandgap of 2.89 eV, total pore volume of 0.298 cm^3/g, a crystallite size and percent crystallinity of 16.9 nm and 76.8% respectively. Under varying experimental conditions; Li/ZNF decontaminated toxic antiseptic 2,4,5-trichlorophenol (TCP) and bacteria-contaminated water. The photocatalytic degradation of 50 ppm TCP by 10 mg Li/ZNF reached 80% after 6 h with a rate constant of 0.0019 min^{-1} at pH 3 and 4 mM H_2O_2. Also, after 60 min under UV-light, 15 and 25 mg of Li/ZNF inhibited 1 x 10^6 CFU/mL of *S. Aureus* and *E. coli* bacteria respectively. Spectral analysis and active species trapping experiments were used to further explore the photocatalytic degradation process. After the fifth cycle, the photocatalyst's recyling efficiency for TCP decontamination only decreased by 14%.



Photocatalysis with immobilized TiO_2 – coated glass rings and UV-A LEDs as a final treatment step of winery wastewater treatment

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The presence of recalcitrant compounds may predominate on winery wastewaters (WW), which can compromise the efficiency of biological treatments and requires the combination of different processes as a pre- or post-treatment step. Heterogeneous photocatalysis with titanium dioxide (TiO_2) has a wide application in agro-industrial wastewater treatment, with the degradation of organic contaminants into H_2O, CO_2 and organic acids [1]. TiO_2 photocatalysis can benefit from Ultraviolet light-emitting diodes (UV LEDs), that have attracted considerable attention as an alternative mercury-free UV source, to become a more sustainable alternative for wastewater treatment purposes [2].

In this work, TiO_2 Degussa P-25 (Evonik) was immobilized on cylindrical glass Raschig rings (d=l=0.5 cm) and used as photocatalyst in the treatment of a bioremediated winery wastewater. Experiments were carried out in a lab-scale batch reactor, which was illuminated with a UV-A LED photosystem.

Using TiO_2-immoblized rings, economic viability of the process could be improved, due to the ease at separating the catalyst at the end of experiments and its reutilization. It was observed that the immobilized TiO_2 can be reused for four times, without any considerable loss of its photocatalytic activity.

The photocatalytic process was particularly efficient in removing total polyphenols of the WW (more than 80% removal). These pollutants were the most recalcitrant to the previous biological treatment and after photocatalysis, the final concentration complies with the legal limit for wastewater discharge (0.5 mg/L).

With the results obtained so far, we conclude that this system shows potential for a small-scale polishing step of WW treatment. Considering the values of suspended solids, BOD_5, total phosphorous and ammoniacal nitrogen, the final effluent also complies with the chemical legal values for water reuse in irrigation purposes. However, for bioremediated effluents with higher concentrations (>200 mg O_2/L and 10 mg total polyphenols/L), the system alone is unpractical and not efficient, considering the slow degradation of pollutants and the lower removals obtained.

Acknowledgements:

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Photocatalytic H_2 generation from H_2S on CdS-ZnS semiconductors

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Abstract - young researcher

Photocatalytic hydrogen production by H_2S splitting offers sustainable energy generation and abatement of environmental pollution, which is energetically more favorable than photocatalytic water splitting. Sulfide-based materials, as photocatalysts, are regarded as good candidates for H_2 evolution due to their excellent solar spectrum response and high photocatalytic activity. The loading of proper co-catalysts that are based on cheap and earth-abundant materials on those semiconductors was shown to play an important role in the improvement of their efficiency.

In our research, we focused on the use of CdS-ZnS composite because of its controllable band gap and excellent performance for H_2 evolution under visible light. We mainly investigated the effect of several parameters on the H_2 production activity of this type of photocatalysts in order to obtain a cost-effective material.

The CdS-ZnS composite with an enhanced photocatalytic activity for H_2 production was synthesized from ammine complexes, then, compounds of Ni-group metals (NiS and Pt) were applied as co-catalyst on its surface. The illuminations were performed using simple LED lamps and the effects of the ammonia content, the hydrothermal treatment and the washing of the catalyst were investigated. It was found that 0.1% of NiS (or Pt) on the surface of CdS-ZnS, could remarkably enhance its photocatalytic activity if this catalyst is not hydrothermally treated. It was also shown that the performance of this semiconductor was not affected by the initial pH of preparation. However, the hydrothermal treatment and the ammonia content were proven to highly influence the rate of H_2 production in this system and so XRD measurements were performed to explain this dependence.

The excellent photoactivity of the CdS-ZnS catalysts for hydrogen generation encourages further investigations to enhance its performance by optimization of the reaction conditions.

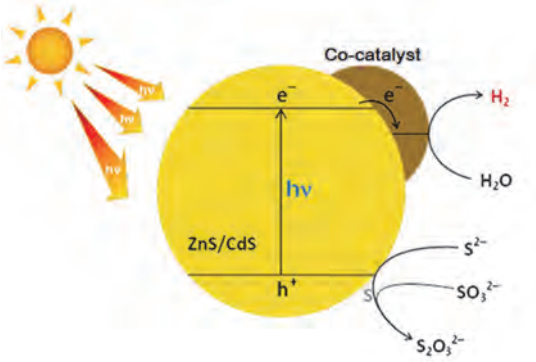

Figure 1. Mechanism of heterogeneous photocatalytic H_2 production

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Photocatalytic treatment of liquid digestate produced from the anaerobic digestion of agro-industrial waste

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Co-treatment of agro-industrial wastewater via anaerobic digestion is an effective process for the exploitation of high organic content materials. Digestates from anaerobic reactors treating these types of wastewaters are widely considered for nutrient recovery applications, in order to reuse ammonia and phosphorus. On the other hand, there is a potential risk of emerging pollutants and pathogenic bacteria that may be present in the digestate, which indicates that further treatment is required in order to reuse it in agriculture. Heterogeneous photocatalysis has been noted as a very efficient technology for removing organic pollutants, and much research has been applied to the use of semiconductor metal oxides due to their high efficiency, stability and low cost.

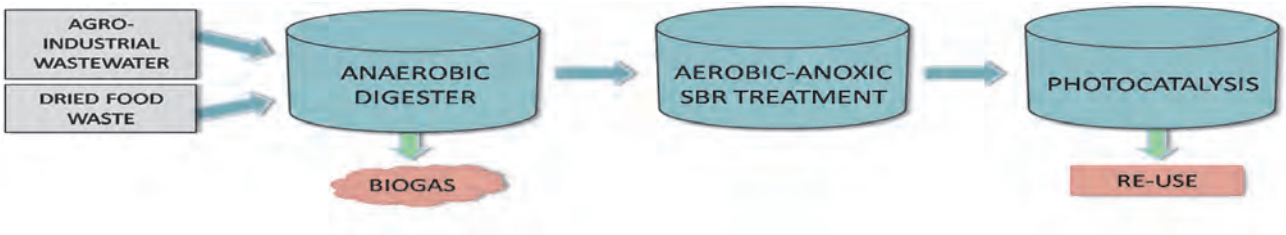

Fig.1 Schematic diagram of the proposed process

The main purpose of this work was to study the post-treatment of the final effluent of a two-stage process (anaerobic digestion – aerobic treatment) with heterogeneous photocatalysis, by monitoring the effect on the aromatic and chromophore groups. Several parameters that affect the photocatalytic rates were evaluated, such as the type of the photocatalyst (TiO_2 or ZnO), the pH of the solution, as well as the addition of an oxidant (H_2O_2, 25 mM).The photocatalytic performance of a synthetic ternary catalyst comprising rGO–ZnO–TiO_2 (2 wt% rGO) was also evaluated in the decoloration of the digestates under ultraviolet light irradiation. Two different types of digestates were evaluated based on the initial mixture of agro-industrial waste (liquid pig manure, cheese whey, olive mill wastewater and dried kitchen waste).

For the first scenario, when TiO_2 P25 was employed, high reduction rates were observed after 3 hr of irradiation, i.e., ~30% for the aromatic and ~60% for the chromophore groups. In addition, when ZnO was used, a lower removal efficiency was observed for both groups (~20% and 40~% respectively). Furthermore, when the synthetic catalyst was evaluated in the presence of H_2O_2, the reduction efficiency reached up to 40% and 80% for the two groups.

Moreover, the addition of H_2O_2 as an oxidizing agent in the reaction medium had a beneficial effect in the removal efficiency. Similar results were obtained for the second digestate for all the tested photocatalysts. Using TiO_2, a 24% removal for the aromatic and 38% for the chromophore moieties was recorded, which increased to 46% and 76% when H_2O_2 was added. In the case of ZnO, the observed removal was 29% and 53% respectively. On the other hand, the use of the synthetic catalyst resulted in a 26% decrease of the aromatic and a 58% reduction of the chromophore groups respectively.

Acknowledgment: "This research has been co-financed by the European Regional Development Fund of the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call RESEARCH – CREATE – INNOVATE (project code:T1EDK-01633)"

Photocatalytic materials for air and water purification - an overview

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The most widely used semiconductor photocatalysts are TiO_2 and ZnO because of their high photosensitivity, photochemical stability, large band gap, strong oxidizing power and non-toxic nature. In particular, anatase TiO2 has been reported as the most extensively used semiconductor photocatalyst for the last 50 years. Recent researches highlight ZnO to show an even better activity than TiO_2 in the photodegradation of some dyes in aqueous solutions. The successful exploitation of such photocatalysts requires the development of techniques for controlling their size, morphology, structural and surface characteristics, as well as efforts to enhance their photochemical response to visible/solar illumination. Until now, there are quite few reports in the literature presenting state of art approaches of use of TiO_2 and ZnO materials onto textile substrates for several applications such as antibacterial [1], deodorizing [2] and UV protection [1,3], and none regarding any systematic approach of direct growth and optimization with respect the textile support. More than that, up to our knowledge, there are only a few available studies in the literature [4, 5] about TiO_2 and ZnO coated textiles used as photocatalytic active support for gaseous compounds decomposition except our previous reports [6]. The present presentation will particularly introduce our recent advances on photocatalytic pure and doped TiO_2 and ZnO onto textile supports and other supports for air and water purification applications.

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Photo-degradation of some landfill contaminants on the surrounding waters

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Abstract

Influences of landfill on the surrounding waters have been studied in Bucharest area. Analytical and spectrometric methods were used to investigate the waters of a canal situated in the neighborhood of the landfill. Dangerous chemical compounds have been identified in water assigned to pollutants resulted from physico-chemical processes of degradation of the landfill wastes. The quick method with gas sensor detection and colorimetric ion identification using commercial Quantofix kit, as well as precipitation with $AgNO_3$ offered preliminary information completed by Fourier Transform Infrared Spectroscopy (FTIR). Pollutants that reached the canal waters either by air (evaporation) or by discharges or through rainwater were analyzed from the point of view of the degree of danger, sources of waste materials, as well as their circuit in the environment. Hydrocyanic acid, nitrites, nitro compounds, sulfites and sulfates, sulfonic tension-active compounds, peroxydes and hyperoxydes, azo-compounds, organic and inorganic acids of high corrosive potential and Fe ions were generally the detected pollutants, each of them with specific harmful potential contributing as well in a cumulative effect to endangering the human health directly or indirectly as environmental circulating contaminants.

Keywords: landfill wastes, hydrocyanic acid, FTIR of water pollutants

Size controlled Ag decorated TiO_2 plasmonic photocatalysts for tetracycline degradation under visible-light

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The TiO_2/Ag plasmonic photocatalysts were successfully synthesized through facile method and silver nanoparticles（Ag NPs）deposited on surface of TiO_2 nanospheres with electrostatic-controlled self-assembly. In this experiment, we synthesized Ag NPs of different sizes by adjusting the molar ratio of silver nitrate to trisodium citrate. The TiO_2/Ag samples exhibited higher photodegradation efficiency of tetracycline (TC) than pure TiO_2 under sunlight owing to the unique surface plasmon resonance (SPR) effect. Detailed analysis based on room temperature photoluminescence (PL), photocurrent and UV–Vis spectroscopy revealed that Ag NPs significantly reduced photogenerated electron-hole pair recombination rate and enhanced visible light absorption. Durability test shows that TiO_2/Ag photocatalyst has stable photocatalytic activity. A possible mechanism of TiO_2/Ag nanocomposites also was discussed.

Keywords：TiO_2/Ag; SPR; Visible-light; Photocatalyst; Tetracycline; Antibiotics;

Size-controlled platinum deposited on titania for enhancement of photocatalytic performance

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Noble metals nanoparticles (NMNPs) have been used for the enhancement of photocatalytic activity of wide-bandgap semiconductors (e.g., titania) for more than forty years (since studies by A. J. Bard [1]), because of hindering of charge carriers' recombination as an electron sink. Moreover, their use as "plasmonic sensitizers" (to activate semiconductors toward visible light (vis)) has recently been investigated, due to ability of vis absorption through localized surface plasmon resonance (LSPR). It should be pointed out that the properties of both titania and NMNPs strongly influence the resultant properties of NM-modified titania, and thus the photocatalytic activity [2-3]. Additionally, sliver and copper could be oxidized causing co-existence of different oxidation states of NMs, and thus forming also coupled oxides that participate in the overall photocatalytic performance [4-5].

In the present study, size-controlled NMNPs (Pt NPs) have been prepared by two methods, i.e., photodeposition and radiolysis. In the case of photodeposition, 500 mg of titania was suspended in 250 ml of 50 vol% methanol solution in the present of H_2PtCl_6 (Pt; 2 wt%) and photoirradiated with the high-pressure mercury lamp (11.3 mW, $\lambda \geq 290$ nm) under anaerobic condition (Ar-pre-bubbling for 15-min to remove oxygen working as an electron scavenger). Moreover, the photodeposition conditions (light intensity, anaerobic/aerobic and different hole scavengers [4]) have been varied to obtain photocatalysts possessing different properties of Pt NPs, e.g., uniform/aggregated, different sizes and morphology (spherical, rod-like). In the case of radiolysis, 100 mg of titania was suspended in 10 ml of 0.1 M 2-propanol in the presence of Pt salt (H_2PtCl_6, $Pt(NH_3)_4Cl_4 \cdot 6H_2O$ or platinum(II) acetylacetonate), bubbled with N_2 for 5 min and irradiated by gamma-ray (γ) radiated for 2 h.It has been confirmed that even slight

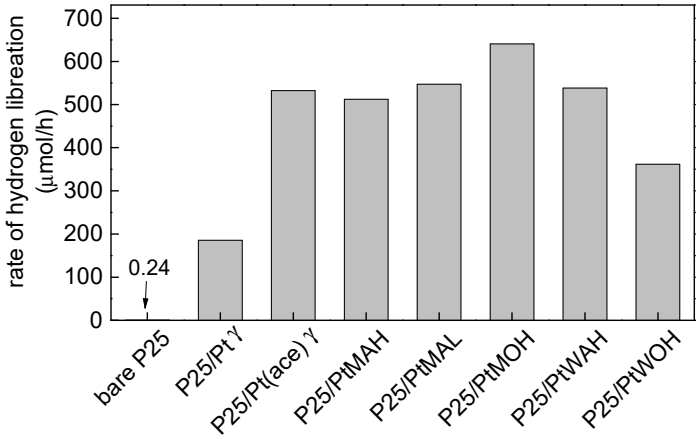

Fig. 1. The photocatalytic activity during methanol dehydrogenation of Pt-modified P25 (commercial titania) prepared by different methods/conditions: γ- Gamma radiation; Pt(ace)- platinum(II) acetylacetonate; M- 50 vol% methanol solution; W-water; A- Ar gas bubbling; O-O_2 bubbling; H- high intensity of photoirradiation; L- low intensity of photoirradiation.

change in the preparation conditions has resulted in significant change in the physical properties, estimated by DRS, XRD, XPS, STEM, TRMC (time-resolved microwave conductivity), and thus in the resultant photocatalytic activity, as exemplary shown in Fig. 1. It is thought that deposition of uniform Pt NPs (fine NPs) is key-factor for methanol dehydrogenation under UV irradiation, whereas aggregation of platinum resulting in broad LSPR peak causes efficient light harvesting, and thus high activity under vis irradiation. Details will be discussed during presentation.

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TiO_2/UV-A mediated advanced oxidation of an emergent water contaminant: toward process enhancement

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Sartans are a class pharmaceuticals which are detected in the water bodies because of their excessive consumption over the world as well as of the rapidly development of the pharmaceutical industry. They are amongst emerging water contaminants because they are not regulated yet by the water framework directive. According to several reports some of these organic molecules are not efficiently eliminated by the municipal wastewater treatment plants (WWTPs) based on activated sludge, so they are continuously released into the aquatic system seriously affecting the development of aquatic and wildlife (Vrinceanu et al., 2019). Hence, today there is an increased demand for the development of complementary highly efficient treatments for their removing before their discharge into the environment order to prevent the water resources pollution.

Advanced oxidation processes (AOPs) and more especially heterogeneous photocatalysis is recognized today as an efficient destructive technique and was successfully applied in many studies for the degradation persistent pollutants. Indeed, it is considered as an attractive water detoxification option because of its ability to mineralize organic compounds into harmless molecules, to operate without pH adjustment, in mild conditions of pressure and temperature, and its saving treatment costs (Rizzo et al., 2009). Therefore, this study focuses on the photocatalytic degradation of pharmaceutic compounds belonging to sartans family using TiO_2 as catalyst and UV-A irradiation conditions. Photocatalytic runs were performed at room temperature, at laboratory scale in a batch reactor (working volume of 1L) using UV-A mercury vapor lamp as light irradiation source. Samples were withdrawn from the reactor at different reaction times and the residual pollutant concentration was recorded with an HPLC system operating under isocratic mode.

According to the results of photocatalytic tests a highest removal of pollutant (about 95%) was achieved after 10 minutes of irradiation for 1.3 g/L of catalyst load and initial pollutant concentration of 6 mg/L. Under these conditions a excellent mineralization yield of 87% was achieved after 2h of irradiation. It was also observed that the removal and mineralization

efficiencies strongly depend on the considered operating conditions such as catalyst type and its concentration, initial pollutant content, solution pH and light intensity. Also, the collected data demonstrated that under all studied process conditions the target molecule was degraded according to a pseudo first order kinetics model.

In summary, this investigation confirmed that UV-A/TiO_2 photocatalysis successfully enhances the degradation and mineralization of the considered drug of the sartans family. The next step of this study is a detailed investigation of reaction intermediates generated during this oxidation process.

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Structural investigations of photocatalytic ZnO nanostructures

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Photocatalysis which it is defined as "the acceleration of a photo-generated electron in the presence of a catalyst" represents a well-known technique with promising applications in the degradation of organic pollutants [1,2]. Up to date, the scientific community made an intensive effort to reduce this problem, taking into account the use of metal oxides. In this sense, zinc oxide (ZnO) gathered interest, due its wide direct band gap of 3.37 eV and the large exciton binding energy of 60 meV are the characteristics that make it a unique candidate for such applications [2]. At the same time, the possibility to tune the ZnO morphology in a large window, from nanoparticles, to nanorods, nanowires or nanotubes it is another aspect that should be mentioned.

In this paper, we provide a thoroughly investigation of ZnO nanostructures using X-ray diffraction. A further understanding of the crystal quality in terms of the mean crystallite size and lattice strain it is achieved using Williamson-Hall plots that make possible a decoupling the size and strain effects from the total peak broadening. Different stages of ZnO formation can be distinguished, namely: complete formation of ZnO, unreacted metallic Zn and unreacted $Zn(OH)_2$, further ascribed with different ZnO morphology as revealed by scanning electron microscopy. In the meanwhile, different size for crystalline domains were calculated, being suggested the relationship between morphology and crystal quality. Our findings are completed by Raman spectroscopy, which showed an evolution of the Raman modes. Finally, the results are correlated to the photocatalytic activity of our samples, studied by means of the reduction of 50 ppm aqueous solution of paracetamol, a well-known pharmaceutical product that has been used as an organic model to probe the photocatalytic performance of photocatalysts.

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Superior Photocatalytic Performance of Ancillary-Oxidant-Free Novel Starch Supported Nano MFe_2O_4 (M = Zn, Ni, and Fe) Ferrites for Degradation of Organic Dye Pollutants

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In this work, for the first time, the effective degradation of MB and MO dyes in an aqueous solution under UV light irradiation on starch-supported nano ferrites without using any supplementary oxidants has been achieved. Nano $ZnFe_2O_4$, $NiFe_2O_4$, and Fe_3O_4 are successfully produced via co-precipitation technique utilizing biodegradable starch for surfactant. XRD patterns reveal a pure spinel phase for all the samples. FTIR spectra confirm the successful embedding of the starch surfactant. SEM micrographs exhibit tiny spherical particles of size 5-8 and 4-6 nm, respectively, for $ZnFe_2O_4$ and $NiFe_2O_4$, but spherical particles of size 8-10 nm and flake-like particles of ~14 nm thick for Fe_3O_4. N_2 sorption studies show type-IV isotherms typical of mesoporous structures. The direct bandgap of these ferrite nanoparticles is 2.03-2.15 eV, related to the metal d-d onsite transfers which are permitted by spin but prohibited by parity. MB degradation of 99 % is achieved in less than 2 h for all the samples, in contrast, MO degradation takes relatively longer irradiation times. The adsorption kinetics suggest that the pseudo-second-order model is better suited to explain the adsorption process of MB and MO by the catalysts. The order of photocatalytic activity assessed from rate constant (k_1 in min^{-1}) values is $NiFe_2O_4$ (0.086) > $ZnFe_2O_4$ (0.077) > Fe_3O_4 (0.069) for MB degradation and $NiFe_2O_4$ (0.029) > $ZnFe_2O_4$ (0.026) > Fe_3O_4 (0.021) for MO degradation. $NiFe_2O_4$ photocatalyst shows supreme effect towards the degradation of both the dyes thanks to its low bandgap and high surface area. All the ferrite catalysts demonstrate high stability with no substantial deterioration of photocatalytic activity even after three cycles. The results of this study endorse that the starch-supported nano-ferrites prepared in this work are potential candidates for the photocatalytic degradation of aqueous solutions of MB and MO. The results of this study are expected to encourage more studies on the direct use of pristine nano-ferrites in photocatalytic degradation of dye pollutants without using any additional oxidants.

Keywords: Oxidant-free Photocatalysis, Organic pollutants; Ferrite Nanoparticles; Starch; Degradation; Bandgap.

Unveiling photocatalytic potentiality of rare-earth metal oxide tethered conductive polymer nanocomposite

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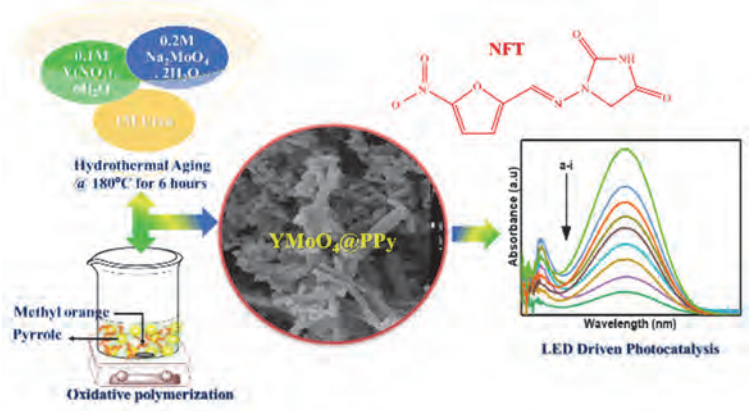
Abstract young researcher

The present work reveals the photocatalytic ability of yttrium molybdate coupled polypyrrole nanocomposite ($YMoO_4$@PPy) towards the removal of nitrofuran-based broad-spectrum antibiotic, nitrofurantoin (NFT) from water sources under the irradiation of light-emitting diode (LED). Here, $YMoO_4$ was hydrothermally prepared while template-driven growth of PPy nanotubes was employed. However, the preparation of composite ($YMoO_4$@PPy) was abetted by facile ultrasonic irradiation. The as-synthesized $YMoO_4$@PPy was subjected to, electron-microscopy to determine the morphology, X-ray diffraction to know the structural configuration, Fourier-Transform infrared analysis to confirm the functional entities, UV-Visible spectroscopy for determining the bandgap, and electrochemical impedance spectroscopy to note its electrical conductivity. The composites (1:1, 1:2, and 2:1 $YMoO_4$@PPy by percentage weight) and the individual counter-parts ($YMoO_4$ and PPy) were then evaluated in a LED-aided photocatalytic system against NFT. It was observed that ~93% of NFT (15 ppm) was mineralized within 80 minutes of reaction by 1:2 $YMoO_4$@PPy (25 mg) catalysts. The reaction kinetics fitted the pseudo-first-order model with an appreciable regression coefficient. Here, the influence of conducting polymer is significant in terms of rapid electron mobility and prolonged charge separation. Also, the minimal blend of rare-earth oxide upholds the economy and real-time application. Therefore, the present work explicitly explored the combination of rare-earth metal oxide interfaced conductive polymerowing to its photo- and electro-intrinsic traits.



Keywords

Photocatalysis; antibiotic degradation; nanocomposite; rare-earth metal oxide; wastewater treatment; conducting polymer

Versatility of cellulosic matrix used for immobilization of synthesized CeO_2 nanoparticles in tailoring the photocatalytic properties of hybrid composites

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Photocatalysis plays a pivotal role in global issues of nowadays, meeting the requirements of sustainable chemistry and green organic synthesis, with applications in a large variety of processes, from organic pollutants mineralization to fine organic reactions, its great benefit consisting in the direct conversion of light energy into chemical energy, ensuring thus a green, sustainable and economic approach to limit the environmental pollution.

The research in this field is very much governed in general on the use of semiconductor materials, and researchers' interest focused mainly on TiO_2, tends to be shifted to other metal oxides and their nanoparticles. Among them, CeO_2 NPs seems to be one of the most active photocatalysts, since the cerium oxide as one of the most reactive rare earth oxides, have a band gap similar to TiO_2 NPs (Eg = 3.19 eV). CeO_2 have a particular outer electron configuration of $[Xe]\ 4f^1 5d^1 6s^2$, that enhance the electron transfer from the adsorbed organic molecules to oxygen species and its price has considerably dropped over the last years, reaching in 2018 a minimum value of 6.36 USD/kg. CeO_2 is a robust and feasible „platform" for the next generation of photocatalysts also due to the reversible shift of the oxidation state between Ce^{3+} and Ce^{4+}, formation of oxygen vacancies in the cubic fluorite structure, high electron transfer capability, long-term stability, and nontoxicity. Unfortunately, the use of inorganic nanoparticles as photocatalysts is drastically limited by their agglomeration tendency, that leads to a decrease of their surface area and eventually of their photocatalytic efficiency, but also in the difficulties arises during their separation and reuse. To overcome these drawbacks, in the literature was emphasized that the use of various polymers as supports for the efficient immobilization of active photocatalytic nanoparticles, could represent a viable solution, due to some unquestionable advantages that the polymeric supports present: resistance to ultraviolet radiations, high durability, chemical stability, and easy availability.

In view of all these information, this study reports the fabrication of a tuneable and flexible reproducible cellulose-based platform for immobilization of surface functionalized CeO_2 nanoparticles intended to be used as photocatalysts under UV irradiation for the degradations of model pollutants (organic dyes and 4-nitrophenol.

Acknowledgement

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Visible-Light Photocatalytic H_2 Production Activity of β-$Ni(OH)_2$-Modified CdS Mesoporous Nanoheterojunction Networks

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Photocatalytic water splitting for H_2 production represents a promising strategy for converting solar energy into chemical fuels.[1] To that end, the development of robust and highly active semiconductor materials is of eminent importance in this field. Transition metal sulfide nanoparticles, such as CdS, have attracted enormous research attention because of their high photon-to-electron conversion efficiency, excellent electron conductivity and low cost. Nevertheless, single-component CdS semiconductors suffer from low charge-carrier separation yield and poor chemical stability. One of the most effective ways to overcome the limitations of charge recombination and anodic photocorrosion in CdS materials is the coupling of CdS with noble metal co-catalysts, such as Pt nanoparticles, which can increase the electron–hole separation yield through the efficient charge-carrier dissociation at the interface of the formed heterojunctions.[2] However, the high-cost and limited availability of Pt hinders its practical application in sustainable H_2-generation technologies. Here, we demonstrate high-surface-area mesoporous networks comprising linked β-$Ni(OH)_2$ modified CdS nanocrystals as highly active noble-metal-free photocatalysts for H_2 generation. Compared to single-component CdS assemblies, Ni-modified materials present a strong enhancement of photocatalytic performance for H_2 evolution under visible light irradiation ($\lambda \geq 420$ nm).[3] By controlling the growth of β-$Ni(OH)_2$ particles, the mesoporous β-$Ni(OH)_2$/CdS heterojunction networks at a 10 wt.% Ni-content reached an outstanding photocatalytic H_2-evolution rate of 1.4 mmol h^{-1}, which is associated with an apparent quantum yield (QY) of 72% at 420 nm in a 5 M NaOH aqueous solution containing 10% v/v ethanol. Notably, this efficiency was found to be comparable with, and even slightly higher, than that of the optimal 5 wt.% Pt/CdS counterpart. Mechanistic studies with UV–Vis/DRS, photoluminescence, electrochemical impedance spectroscopy, and photocatalytic evaluation experiments suggest that the improved photocatalytic performance arises from the strong electronic coupling and charge-transferred states at the p–n β-$Ni(OH)_2$/CdS heterojunctions. This work not only presents the possibility of using these β-$Ni(OH)_2$ modified CdS mesoporous assemblies as a viable hydrogen evolution photocatalyst, but also can offer new insight for the development and in-depth understanding of noble-metal-free photocatalysts for efficient solar-to-chemical energy conversion.

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Visible Light active Bismuth ferrite embedded TiO_2 nanocomposite structures for mixed dye mineralization by photocatalysis: A strategy to harness solar energy for wastewater remediation

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Harnessing solar energy to treat effluents from industries in order to mineralize the organic pollutants by photocatalysis demands the use of photocatalysts which are visible light active.

In the present study, Bismuth ferrite embedded TiO_2 (BFO/TiO_2) nanocomposites have been synthesized with BFO (prepared by co-precipitation method) to Ti molar ratio of 1:2. BFO/TiO_2 nanocomposites are crystalline, oval shaped and monodispersed with the average hydrodynamic diameter of 42 nm.

Transmission electron microscopy revealed that BFO nanoparticles have an average shorter dimension of 13.4 nm and longer dimension of 15.5 nm and are embedded in TiO_2 matrix with the average coating thickness of 4.8 nm. The apparent band gap energy of BFO/TiO_2 is 1.4 eV. BFO/TiO_2 nanocomposites were used for the degradation of dyes from mixed dye aqueous solution containing three azo dyes, *viz.* Acid yellow-17 (AY- 17), Methylene Blue (MB), and Rhodamine- B (Rh-B) dyes under visible light irradiation. The BFO/TiO_2 nanocomposites exhibited good photocatalytic activity under visible and solar light. Around 92% of MB dye, 73.9% of AY-17 and 68.3% of Rh-B dyes were degraded in 210 min from the mixed dye aqueous solution. Chemical Oxygen Demand (COD) removal of 72% could be achieved by photocatalysis confirming the mineralization of dyes. The COD removal kinetics followed first order model with the rate constant of 0.006 min-1. BFO/TiO_2 nanocomposites exhibited superior visible light activity compared to BFO or TiO_2 (Degussa P25) nanoparticles. The BFO/TiO_2 nanocomposites have been proven to be promising in remediation of wastewater contaminated with mixture of dyes by photocatalysis.

Keywords: Bismuth ferrite; Dyes; Kinetics; Nanocomposites; Photocatalysis; Titanium dioxide

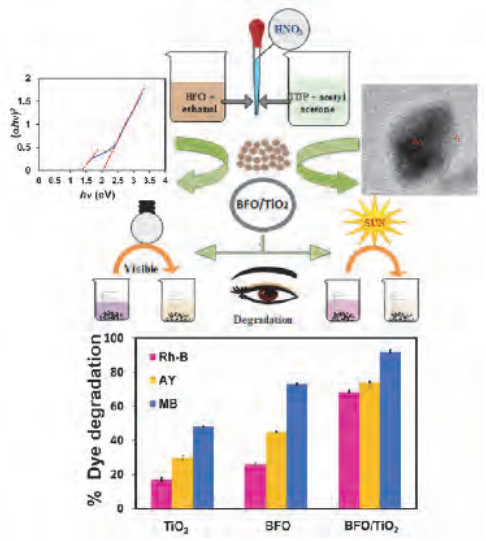

Figure: Graphical Abstract

ZnO-(r)GO composite thin films for photocatalytic applications

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This study is focussed on the development of ZnO-GO (graphene oxide) and ZnO-rGO (reduced graphene oxide) composite thin films designed to be used in the advanced wastewater treatment through photocatalytic degradation of the organic pollutants, at low concentrations.

Thin films based on ZnO – (r)GO composite layers were deposited using combined sol-gel and room temperature spraying techniques. The ZnO-GO composite sol was synthetised by mixing, at 60ºC for 1h, a precursor system containing zinc acetate (c = 0.5 mol/L), GO (added as aqueous dispersion), isopropanol (as continuous medium) and monoethanol amine (as stabilizer). The GO dispersion was added in an appropriate amount to insure up to 5% GO (%wt) in the thin films. The ZnO-rGO composite sol was obtained in similar conditions with the rGO derivative added in the sol as ethanolic dispersion.

After aging for 48 h at room temperature in open atmosphere, the composite sols were diluted with isopropyl alcohol and sprayed onto glass plates previously coated with a thin film of ZnO (deposited by spray pyrolysis deposition).

The ZnO/ZnO-(r)GO thin films were further thermally treated at 150^0C to support an organized structure without degrading the graphene derivatives oxidation.

The thin film structure (XRD), surface morphology and composition (SEM, AFM, EDX) were investigated; the results prove the incorporation of the (r)GO in the ZnO matrix and the formation of composite thin films with dendrite-like morphologies, containing ZnO and randomly distributed carbon. The carbon content at the thin films surface is in good agreement with the (r)GO amount added in the sol synthesis proving that the temperature was well selected in the process.

The photocatalytic properties and stability of the ZnO/ZnO-(r)GO thin films were tested using methylene blue (MB) 10 ppm solutions (standard organic pollutant) and radiation at low irradiance values with different spectral composition: solar simulated radiation (UV + VIS, G=55 W/m^2) and UV radiation (G=10 W/m^2), up to 8h. Experimental tests were run in similar conditions, but without irradiation (in dark) to outline the role of the adsorption in the pollutant removal process.

Promising methylene blue photodegradation efficiencies of 22…30 % were recorded after 8h of UV+VIS irradiation, values that are higher (up to 10 %) compared to the corresponding efficiencies when only UV (G=10 W/m^2) radiation was applied. This outlines that the investigated thin films are Vis/(solar)-active photocatalysts. The Vis-activation becomes more significant as the (r)GO content increases in the thin film.

The variation in the thin film transmittance and the changes in the surface properties (morphology, RMS) before and after photocatalysis were used to evaluate the thin films stability. Good stability corresponds to the thin films containing 3% of GO or 3% rGO as confirmed by the average variation in transmittance before /after photocatalysis (less than 20%), the increase in the surface roughness (less than 50 nm) and the small modifications of the surface morphology.

These results indicate that the composite thin films with 3% (r)GO content can be recommended for testing at pilot plant scale targeting future applications in the advanced treatment of wastewaters loaded with organic pollutants at low concentration (in the ppm range).

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POSTERS

3D printed nanocomposites for energy and environmental applications

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In this study we employ the 3 dimensional (3D) printing technology, in order to fabricate large scale 3D structures, dedicated for energy and environmental applications.

Lately, 3D printing technology has gained a lot of interest in various research fields, such as medicine, chemistry and materials science, as an alternative, trendy and effective route for production of 3D printed samples. Especially in polymers, widely known polymers such as polyvinyl alcohol (PVC), polystyrene (PS) acrylonitrile butadiene styrene (ABS) and poly lactic acid (PLA), can easily be printed employing the so-called fused deposition modeling (FDM) process. According to this procedure, the chosen polymer, which have been mechanically transformed into long flexible wires, called filaments, is heated above its melting point and then it is extruded through a narrow nozzle form a 3 dimensional shape by layer-by-layer deposition on a platform. Polymeric structures of various sizes, densities and functionalities can be produced in such way, by selecting appropriate starting materials.

There are plenty of commercially available polymer-based filaments for countless applications, such as conductive, magnetic, flexible filaments. In most cases such filaments are produced by blending a polymer with nanoparticles of inorganic materials. However, it becomes prudent to produce custom-made filaments, consisting of materials with dedicated properties. Considering that the nanoparticles keep their properties unaffected, after the blending with the polymer matrix the produced filament could exhibit corresponding functionalities.

Considering all the above, we fabricate 3D polymer nanocomposite structures, of commercially available ABS and PLA filaments, enriched with various carbon structures, namely graphite nanofillers, carbon nanotubes and graphene oxide nanosheets, and we studied them regarding their electromagnetic shielding efficiency in the C-band of the electromagnetic spectrum (3.5–7.0 GHz), which is typically used for long-distance radio telecommunications. Through this study, it is evidently proven that 3D printing technology can be effectively used to prepare operational shields, for electronic device applications.

Furthermore, we fabricate polymeric filaments, consisting of PS and ZnO or TiO_2 nanoparticles and then we used them to construct 3D printed photocatalytic structures. The produced structures exhibit an efficiency of 70% after five cycles of use in a 20 ppm Methylene Blue aqueous solution, under UV irradiation. Thus, it is evidently shown that 3D nanocomposite structures show promising photocatalytic properties, for potential real – life environmental applications.

AMC-COMSOL: the new finite element technique to increase solar cell conversion

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AMC (Active Magnetocaloric Cooling) is the promising revolutionary cooling technology aimed to reduce energy consumption and greenhouse gases, addressing this way the concerns of global warming and human health. Developing new technologies require multiple experimental trials and theoretical analyses. Finite element method is one of the most suitable options for setting up a model of simulation. We used COMSOL Multiphysics software to build up a mathematical and simulation model for the cycle of AMC to determine the timing and to improve the effectiveness of the device. The simulation consists of three steps. The first and the second step consist of heat transfer in solids and fluids. The third step is a magnetic simulation which analyzes the effects of the magnetic field on gadolinium. Pumping frequency optimization is analyzed with parametric sweep. The lowest temperatures induced in both gadolinium and in fluid are noticed at 33 Hz pumping frequency. Map of magnetic flux density at constant magnetic field is analyzed to search for clues to improve the refrigeration device. The model can be extended to study influence of the variation of different parameters involved in the process, being designed as a flexible model.

Keywords: Active Magnetocaloric Refrigeration, COMSOL, environmentally friendly, gadolinium

Considerations about the determination of the band gap from diffuse reflectance spectroscopy

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The determination of the band gap energy of semiconductors is important for the understanding of the production of the electron/hole pairs under the light irradiation, which, in the case of photocatalytic materials, are related to their properties and efficiency. The photoexcited electrons and holes are good reductant and powerful oxidant species, respectively. As consequence the free radicals formed can to degrade, after a sequence of redox reactions, various pollutants present in water or air. Diffuse Reflectance Spectroscopy (DRS) is a technique frequently employed to study the optical properties of solids. In this context, the Kubelka-Munk model (K-M model) [1] has been extensively applied to investigate the light scattered diffusely from the surface of semiconductor materials in the form of powders including composite materials. However, in some papers published recently, including some in prestigious journals in the field of Materials Science, it is possible to perceive some inconsistency when the subject matter is the K-M model. Specifically, these problems consist in interpreting the Kubelka-Munk function, $F(R)$, as the absorption coefficient [2,3], assigning an arbitrary unit for the dimensionless $F(R)$ [4–6] or even confuse the K-M function with the equation that frequently is used to estimate the band gap energy [7–9]. These oversimplified or even incorrect interpretations may confuse the readers concerning the applicability and validity of the K-M model. Therefore, the main objective of this work is to explain all the necessary steps to obtain and interpret $F(R)$, as well as to apply it for the determination of the band gap from DRS data of a polycrystalline powder of the wide-gap semiconductor TiO_2. Thus, with this work it is expected to help researchers who are starting their studies involving the determination of the band gap from DRS data and to clarify the procedure to those who could be confused due to the various drawbacks previously identified.

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CdSe Quantum Dots insertion effect on the alpha-keratin PLD-thin films

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Suspensions of CdSe nanocrystals in hexane were produced by colloidal synthesis from Cadmium oxide and selenium as precursors. Quantum Dots were synthesized successfully at different times with a change of color in visible and even more evident in UV. The change in color is assigned to a change in size and shape of the nanocrystals. The Quantum Dots were characterized using non-invasive spectroscopy in UV-Vis and with Laser Induced Fluorescence. Three of the samples of QDs in suspension were spread on thin layers of alpha - keratin obtained by pulsed laser deposition (PLD) on hemp fabric and glass substrates. In order to evaluate the processes, suspensions were also tested on the hemp fabric without keratin film. Sorption, dispersion and physico-chemical processes in the keratin thin films and in the hemp fabric were studied by Optical Microscopy, Scanning Electron Microscopy (SEM) coupled with Energy Dispersive X-Ray Spectroscopy (EDS) and Fourier Transform Infrared Spectroscopy (FTIR). Study of Quantum Dots is of great interest in order to develop new nanotechnologies where their optical properties are required, such as solar cells, but also medical devices. Quantum Dots are also important for their photocatalytic role in chemical processes driven by light, such as water decomposition to obtain Hydrogen as “solar fuel”. This work is part of a larger study to investigate different means to produce QDs and their insertion in different materials and also analysis of QDs behavior under different conditions.

Keywords: CdSe Quantum Dots, alpha keratin thin films, colloidal synthesis, hemp fabric.

Chemical processes induced by light on the AuNP-citrate surface

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Previous studies in fungal cell cultures, incubated with AuNP-citrate and irradiated in the visible light, showed an increased level of reactivity and low cytotoxicity. The control of reactive oxygen species produced by AuNP exposed to green light radiation, by modifying the irradiation time, is the purpose of this study. Colloidal AuNP suspensions were prepared according to adapted Turkevich method by reducing precursor gold compounds with sodium citrate. Sample irradiation was carried out with green light for various exposure time. Sample characterization was performed using spectral analyzes UV-Vis, TEM and FTIR. It was found that about 17 nm diameter particles dominate in all samples – as resulted from Surface Plasmon Resonance absorption band, characteristic to gold nanoparticles. FTIR spectra of the samples irradiated at 60 minutes, 80 minutes and 100 minutes evidence completing the reaction between tetrachloroaurate (III) trihydrate ($HAuCl_4x3H_2O$), sodium hydroxide (NaOH) and citrate decomposition after 100 minutes up to itaconic and citraconic anhydrides. A simulation was conducted in COMSOL Multiphysics software, where a mathematical model has been added to the Heat Transfer module for the irradiation at 50 W and visible light of 520 nm wavelength of AuNP in aqueous solution 50g/l. The results confirmed that there are conditions for citrate decomposition into dehydrated acids and itaconic and citraconic anhydrides.

Keywords: AuNP-citrate, green light irradiation, COMSOL, Laser Induced Fluorescence

Co_3O_4-Bi_2O_3 heterojunction; An effective photocatalyst for photodegradation of rhodamine B dye

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Recently, the research on development of visible-light-active photocatalysts for photodegradation of organic pollutants has got much attention. Therefore, this study reports the synthesis of Co_3O_4-Bi_2O_3 heterojunction as visible-light responsive photocatalyst for photodegradation of rhodamine B dye. The Co_3O_4-Bi_2O_3 heterojunction was synthesized by coprecipitation method and characterized by XRD, EDS, SEM, TGA and FTIR. The as prepared Co_3O_4-Bi_2O_3 heterojunction was utilized as photocatalyst for photodegradation of rhodamine B dye using a 100 mg/L solution. It was observed that Co_3O_4-Bi_2O_3 showed best catalytic performance with ~92% degradation of rhodamine B dye than Co_3O_4 and Bi_2O_3 with 14 and 34% removal of rhodamine B dye, respectively (Figure 1). The rate constant for Co_3O_4-Bi_2O_3 catalyzed photodegradation of rhodamine B was 6 times and 3 times higher than rate constant for Co_3O_4 catalyzed and Bi_2O_3 catalyzed photodegradation of rhodamine B, respectively. The pH 8 was found as optimum pH for Co_3O_4-Bi_2O_3 catalyzed photodegradation of rhodamine B dye.

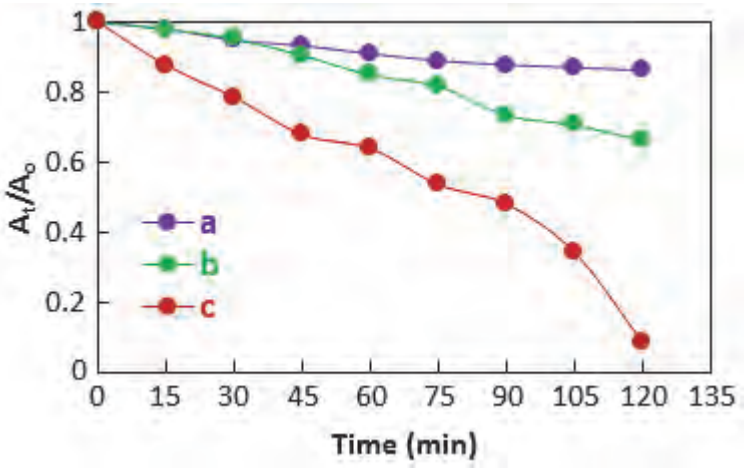

Figure 1 Photocatalytic activity of Co_3O_4 (a), Bi_2O_3 (b) and Co_3O_4-Bi_2O_3 (c) towards photodegradation of rhodamine B dye

Keywords: Co_3O_4-Bi_2O_3, Rhodamine B, Photodegradation

Core-shell particles with thermo-responsive wetting characteristics obtained by photo-mediated suspension polymerization

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The aim of this study consisted in the synthesis and application of a perylenediimide (PDI) based photo-initiator for the fabrication of polymer particles through a photo-mediated reversible deactivation radical polymerization[1,2]. The strategy involved the synthesis of a PDI derivative bearing a reactive tertiary carbon substituted with bromine which was employed in the photo-mediated suspension polymerization of methyl methacrylate. The obtained particles were subsequently used for the surface surface-initiated polymerization of a hydrophilic monomer (N-isopropyl acrylamide) to obtain a thermo-responsive shell. The core-shell morphology of the polymer particles was confirmed by SEM analysis. Contact angle and dynamic light scattering measurements (DLS) were performed at different temperatures to assess the modification of the particle size and temperature effect on the wetting properties. The thermal stability of the polymer particles was investigated by thermogravimetric analysis.

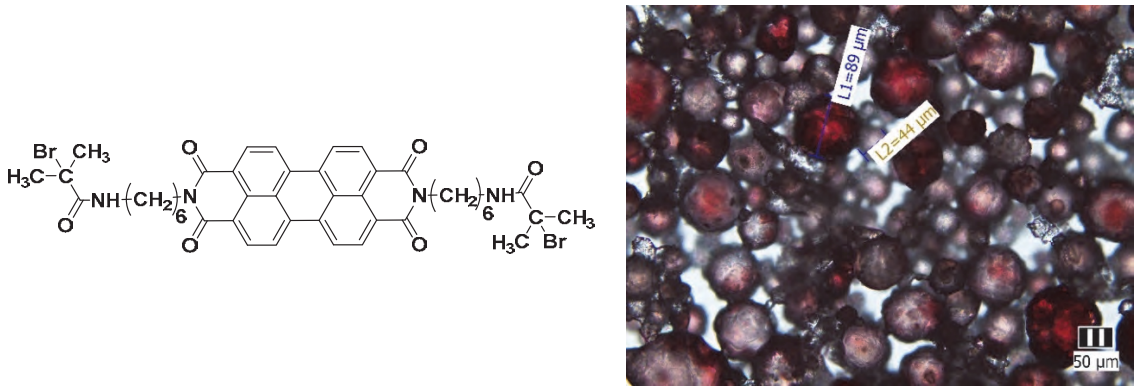

Figure 2. Chemical structure of the photoinitiator PDI derivative and optical microscopy images of PMMA particles

Acknowledgement

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Crystal Growth and Optical Properties of $CH_3NH_3PbX_3$ (X = Cl, Br, I) of Halide Perovskite Single-Crystals

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Halide perovskites AMX_3 (A^+ = Cs, CH_3NH_3 or $HC(NH_2)_2$, M^{+2} = Pb, Sn or Ge and X^- = Cl, Br or I) are amongst the leading emerging materials in the past decade towards optoelectronic and environmental applications, including devices such as solar cells, light-emitting diodes and hard radiation detectors. What makes these semiconductor materials so attractive for optoelectronic devices is their superb absorption across the visible and near-infrared region (E_g = 1.1-3.0eV) and their high charge-carrier mobility and long charge-carrier diffusion lengths. In most cases, the materials have been studied primarily in the form of polycrystalline thin-films but recently a new trend involving the study of single-crystal devices has been proposed[1]. This approach offers significant benefits in terms of device performance, such as higher mobility and electrical contact uniformity, but in order for this approach to be efficient the quality of the crystals need to be optimized.

In this work, we will present the crystal growth of the $CH_3NH_3PbX_3$ (X = Cl, Br, I) family of single-crystals, grown using a wide variety of crystallization techniques, such as the solution temperature lowering (STL), the inverse temperature crystallization (ITC), the anti-solvent vapor-assisted crystallization (AVC). The quality of the as-grown and cleaved crystals was evaluated by X-ray diffraction, whereas the optical properties were measured as a function of temperature to estimate the excitonic and the temperature activated processes occurring in this class of semiconductors. Our findings provide new insights on the physics of these model systems that will aid in the development of efficient devices at room temperature.

CCS acknowledges support from the Special Account for Research Funding of the University of Crete under grant numbers KA10330 and KA10652.

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Current Challenges and Recent Development in Green Synthesis Based Nanomaterials for Energy Applications

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The current economic growth paradigm, which is based on ever-increasing resource consumption and pollution emissions, cannot be maintained in a world with scarce resources and ecosystem capability. The idea of the "green economy" has provided an incentive to change how society approaches the relationship of the environmental and economic spheres in this context. The associated idea of "green nanotechnology" aims to utilize nano-innovations in materials science and engineering to produce products and processes that are energy efficient as well as economically and environmentally sustainable, to allow society to develop and maintain a green economy. This segment is anticipated to affect a wide range of industries, including energy production and storage, clean-tech, and construction, and related infrastructure. These strategies can provide opportunities to reduce raw material trading pressures, strengthen power delivery systems to make them more effective, productive, and safe, and use exotic water sources or nano-enabled construction products, all of which would improve biodiversity and socioeconomic conditions. Green synthesis refers to the use of plant and other natural resource reduction and stabilization agents to manufacture nanomaterials. The variations in bio-reduction agents used for synthesis are used to manufacture nanoparticles (NPs) with distinct forms, sizes, and bioactivity. The process of synthesis does not involve the use of excessively poisonous chemicals or high energy consumption. The main focus of the current review is on the widespread NP production through green synthesis for energy applications. Even so, the advantages of using nanomaterials in green products and processes could come with adverse impacts on the environment, human health and safety, ethical and social concerns, and customer/market approval instability. As a result, our goal is to investigate the connections between green economy core principles and opportunities for implementing nano-applications in this area, as well as to critically analyze their major obstacles, especially in terms of the effect they may have on the health and safety of employees in this innovative sector. These were primarily due to the unknown hazardous properties of nanomaterials, as well as the challenges in characterizing exposure. This evaluation, interestingly, recommends action plans for risk identification, management, and communication.

Data-informed simulations for gold nanoparticles for energy applications

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Gold nanoparticles are widely used in energy materials. Fuel cells, hydrogen storage, batteries, solar energy conversion are some of the fields where gold nanoparticle use shows great

promise and presents several challenges. The shape of nanoparticles plays a key role in these applications as it determines the energies of quantum confinement and of surface plasmons, as well as the number and type of active sites for adsorption of ligands and catalysis.

The equilibrium shape of metal particles is the polyhedron that minimizes the total surface energy. Such shapes are routinely modeled using variations of the Wulff construction [1]. At the nanoscale, edge energy becomes important as the fraction of atoms at edges of nanoparticles cannot be neglected. We present a systematic method for calculation of edge energies based on atomistic simulations of high-symmetry nanoparticles. We derive an expression for the total energy of the nanoparticle that includes contributions from bulk, surface and edge atoms. We use this expression to fit the energy of nanoparticles as a function of the number of atoms and derive bulk-, surface- and edge energies. For the calculation of total energy, we employ a variety of interatomic potentials and first-principles Density-Functional-Theory (DFT) calculations. Finally, we discuss electronic properties of these nanoparticles in comparison to continuum models [2].

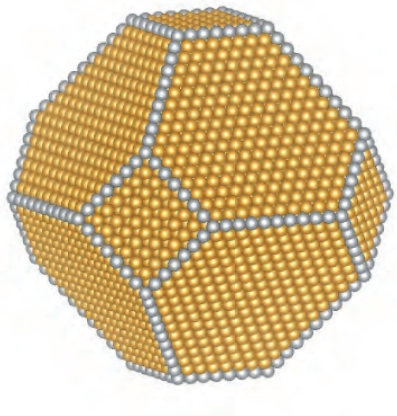

Figure 1: Atomistic model of a typical gold nanoparticle used in simulations.

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Development of carbon adsorbents from industrial pyrolyzed biowaste by-products under varying conditions of $ZnCl_2$ and H_2O_2/HNO_3 activation

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The waste management concerns have motivated agricultural producers to consider the decentralized conversion of biowaste for renewable energy, bio-fuel, and value-added solid by-product generation. During all types of pyrolysis, the carbohydrate components from biomass are broken down following a complex cascade of aldol reactions, cycloadditions, and condensations, carbon-rich solid by-products are obtained. Industrial by-products are intermediate consisting of mainly stable aromatic forms of organic carbons. These renewable sources with high carbon and low ash contents are very favorite raw materials for the production of carbon adsorbents with good features.

In the present work, by-products were obtained from sunflower seed husks by employing in energy plant industry pyrolysis, and its potential for adsorption applications was evaluated. To demonstrate the suitability of these by-products to obtain adsorbing carbons thermal treatment processes under optimized conditions: simple carbonization (or devolatilization) at 600-800 °C, by further chemical activation with $ZnCl_2$ or H_2O_2/HNO_3. The best scheme to develop active carbon materials was assessed by their surface area and porosity characteristics, and chemical composition.

Sunflower seed husk by-products generated in the power plant industry are used as low-cost precursors for future adsorbents. The results of elemental analyses are shown that by-products contained approximately 70% of carbon. Thus, industrial by-products are carbon-rich contaminated biochars. The initial biochars show a weakly developed porous structure and very poor surface chemistry (~ 20 m^2/g). Previous experience demonstrated that temperatures around 600 °C are efficient to produce maximum development of porosity, although carbonization of the material may be incomplete including after carbonization. The biochars derived from sunflower biowastes by H_2O_2/HNO_3 activation were converted to activated carbons with a high surface area and developed porosity. The predominance of meso- or micropores in the obtained porous materials depends on the impregnation ratio of the H_2O_2/HNO_3 activating reagents and biochars, as well as the temperature treatment. The EDX results showed that the biowastes after $ZnCl_2$ activation were contained a high concentration of Zn(II) in the sample. However, the $ZnCl_2$ activation was less effective than H_2O_2/HNO_3. This result was probably due to the complexation reaction of Zn(II) with lignocellulosic components of by-products.

Methylene blue (MB) dye was selected as the target contaminant to evaluate the adsorption capacities of developed materials. The concentration of MB nearly unchanged in the presence of by-products alone, indicating the removal capacity was limited without washing and activation. When using the chemical activation, the removal of MB was accelerated. The samples dominated by micropores exhibited superior dye molecules adsorption capacity, as compared to the samples with higher percentage mesopore volume. This observation could be attributed to the larger absorption capacity as well as additional quantities of active sites for H_2O_2/HNO_3 activated samples. The removal efficiency of MB increased with augment of OH^- concentration and this phenomenon was more attributed to electrostatic interaction. More than 99% of MB could be removed from 15 mg/L solution at an activated sample dosages of 2.5 g/L. Therefore, the prepared activated carbons can be effectively used as effective adsorbents for the removal of organic compounds from an aqueous solution.

First-principles calculations for Mn-doped ZnO

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ZnO is one of the most popular materials for light-matter interaction applications, including photocatalysis. One of the main advantages of ZnO for such applications is that it possesses a wide band gap which is direct, located at the Γ point of the Brillouin zone.

Surface doping allows for tailoring carrier concentration while preserving the superb electronic structure of the bulk material and it will modify adsorption energies and activation energies for catalysis. Moreover, surface doping can alter the workfunction of the material and allow it to be tuned for specific photocatalytic applications.

We present first-principles electronic structure calculations for Mn-doped ZnO. We consider various dopant concentrations at the out-most (surface) layer of Zn atoms, while the interior of the material is kept at the ideal wurtzite structure. For each system, we calculate surface energy and surface workfunction. We discuss trends in surface stability and surface electronic structure of this material, as well as its applications in photocatalysis.

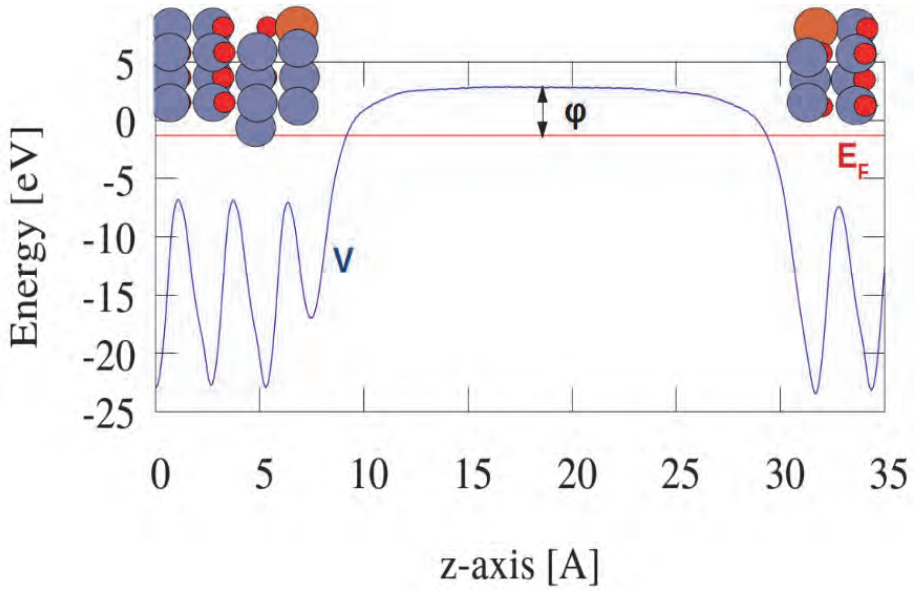

Figure 1: Electronic potential energy as a function of distance from the surface for a periodic simulation of Mn-doped ZnO(0001) slabs. Red, gray and orange spheres represent O, Zn and Mn atoms, respectively. The local potential of the slab (V), Fermi energy (EF) and workfunction (φ) are shown.

The work of AD and NRV was supported by the Research Committee of the Univeristy of Crete (Grant KA10136).

Effect of Sputtering Voltage on the Photocatalytic Activity of Sputtered Silver Nanoparticle Thin Films

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Silver nanoparticle (Ag NP) thin films are widely used in electronic devices, food packing, textiles, medical equipments etc due to their outstanding plasmonic and antibacterial properties. In this work, we have studied the effect of sputtering voltage on the structural, optical and photocatalytic properties of Ag thin films fabricated on glass substrates via DC magnetron sputtering technique. The films sputtered at a voltage of 250 and 275 V are observed to be amorphous while that sputtered at 300 V is partially amorphous. The diffraction peak corresponding to the (111) plane confirms the formation of cubic phase of the Ag thin films. An intense and narrow surface plasmon resonance (SPR) peak is observed at 250 V which becomes broader with further increase in sputtering voltage. The photocatalytic activity of the Ag films sputtered at different voltages is studied using the rhodamine-B dye under UV-visible illumination of 15 minutes. The film sputtered at 250 V exhibits an optimum photocatalytic efficiency of 19 % with a rate constant of 0.016 min^{-1}.

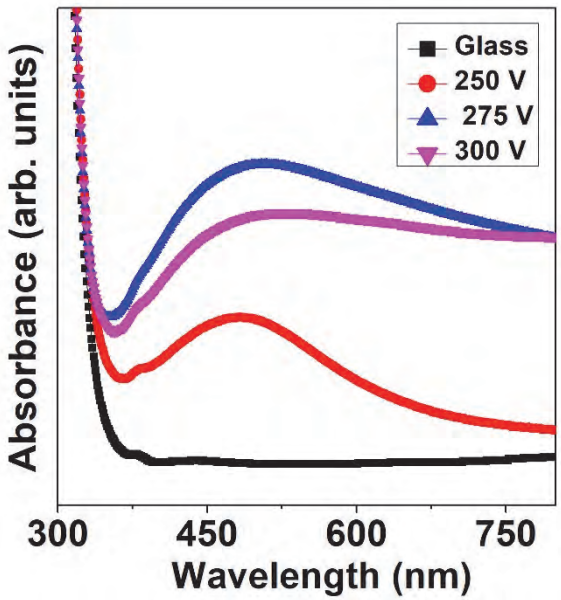

Figure: Absorbance spectra of Ag thin films sputtered at different DC voltages.

Enhanced Photocatalytic Degradation of Dichlorvos using doped TiO_2 catalysts

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Among advanced oxidation processes (AOPs), the photocatalysis is considered as one of the economic, energy-efficient, and clean technology for the removal of organic pollutants. It allows complete mineralization of the organic pollutants into environmentally neutral compounds, such as CO_2 and H_2O, with reactions occurring at room temperature at relatively low-costs. Several types of photocatalysts are available but titanium oxide (TiO_2) is considered as one of the most promising photocatalysts due to its low-cost, non-toxicity, high oxidation efficiency, high photo stability, chemical inertness, and environment-friendly nature. However, the absence of visible light activity (VLA) in TiO_2, resulting from a wide bandgap (3.0-3.2 eV), limits its practical applications as a photocatalyst. Recent reports indicate that doping (adding impurity) TiO_2 with an appropriate anion/cation would result in enhancement in visible light sensitivity of this photocatalyst for the desired application.

Therefore, in the present study, TiO_2 photocatalyst doped with boron (B), and cerium (Ce) and co-doped with both B and Ce were prepared. Then, the efficiency of the prepared photocatalysts was evaluated on the basis of degradation of Dichlorvos (DHV). DHV is a Class Ib (highly hazardous) insecticide, commonly used in developing countries, which is very harmful to aquatic organisms especially fish as it causes damage to the metabolism of the organism, which leads to their death. This work is focused on the correlation of photo-physical and physico-chemical properties of developed catalyst in relation to DHV degradation with them. To the best of our knowledge, no comparative study on the effects of B and Ce doping and co-doping in TiO_2 for photocatalytic degradation of DHV have been reported so far.

Pure TiO_2, B doped, Ce doped, and B-Ce-co-doped TiO_2 nanoparticles were prepared with different content of B and Ce, using a facile, one-step, sol-gel method. The modified catalysts were characterized by N_2 physisorption, X-ray diffraction (XRD), UV-Vis diffuse reflectance spectroscopy (DRS), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), Scanning electron microscopy equipped with energy dispersive X-ray (SEM-EDX), and Fourier transform infrared spectroscopy (FTIR) techniques. The photocatalytic performances of B and Ce doped and co-doped TiO_2 were investigated for the degradation of DHV in aqueous solutions.

After B and Ce doping and co-doping, the optical absorption edge of the catalysts shifted towards the visible region when compared to pure TiO_2. This shift resulted in the lowering of band gap energies of B (2.95 eV), Ce (2.31 eV) doped and B-Ce-co-doped (2.27 eV) TiO_2 samples. The XRD results revealed that the anatase phase dominates in all B and Ce doped and

Co-doped TiO_2 samples. However, the rutile phase and CeO_2 phase were also formed progressively with an increase in dopant (B/Ce) loadings. N_2 physisorption study indicated that Ce dopant induces an increase in the surface area of TiO_2, whereas B doped and B-Ce-co-dopants caused a reduction in surface area. The results of degradation experiments (under optimized conditions) confirmed that photocatalytic activities of B-Ce-co-doped TiO_2 were higher for degradation of DHV as compared to pure and B or Ce singly doped TiO_2. The obtained results suggest that the presence of both the dopants (B and Ce) synergistically promotes the photocatalytic activity compared to pure and single doped (B/Ce) TiO_2

Evans blue photodegradation by novel samarium Doped zinc aluminium spinel ferrites

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The drinking water quality is our responsibility for the generations to come. Unfortunately, by the activity of various industrial branches or household activities, the water resources are strongly polluted with large amounts of organic contaminants [1]. In this context, photodegradation processes represent a suitable alternative for the mineralization of organic pollutants [2].

This study focuses on the synthesis and physico-chemical characterization of new samarium-dopped spinel ferrites with photocatalytic properties, applied in Evans Blue dye photodegradation. The prepared ferrites, with the following general formula: $ZnAlFe_{1-x}Sm_xO_4$ (x=0; 0.02; 0.04; 0.06; 0.08), were dopped with samarium in different ratios. The photodegradation performance increased with samarium content up to 0.06 and then decreased (**Fig. 1**).

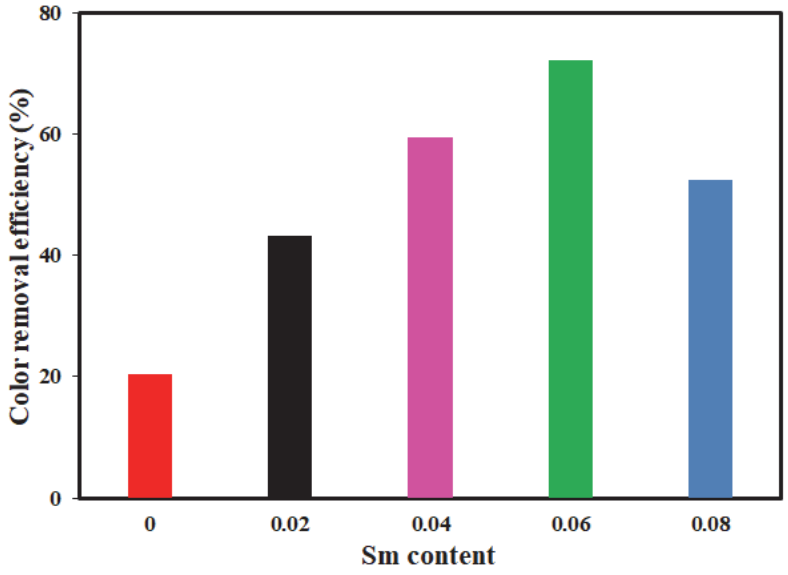

Fig. 1. *Color removal efficiency after 240 min of photocatalytic reaction*

In order to explain such behaviour, the characterization of materials was carried out by appropriate techniques, such as: Fourier transform infrared spectroscopy (FT-IR), X-Ray Diffraction (XRD) and transmission electron microscopy (TEM).

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Fabrication of $CH_3NH_3PbI_3$ perovskite solar cells using the two-step deposition method

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Halide perovskites have monopolized the solar cell research on emerging materials in the past decade given their ability to produce inexpensive, high efficiency thin-film solar cells. Several methods have been developed to date, with more complex compositions and more elaborate device engineering methods yielding a record power conversion efficiency PCE = 25.5% *(1)*. Despite their superb performance, these devices suffer from long-term stability issues, often due to the instability introduced by the presence of secondary phase present in the films. To address this issue, we re-investigate one of the earliest deposition methods for perovskite thin-film deposition; the two-step sequential deposition method *(2)*, originally developed by M. Grätzel and co-workers. Among the advantages of the method allows for the better control of the growth of the crystallites, leading to a better material quality and enhanced surface morphology.

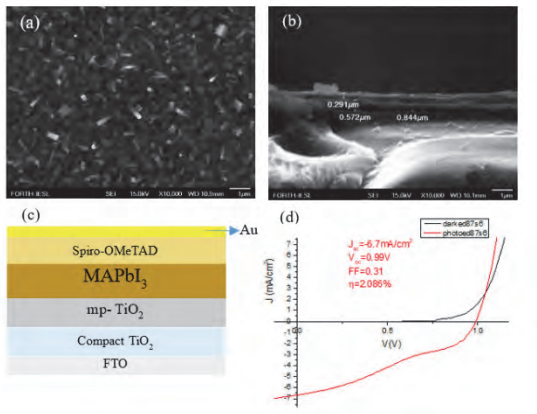

Figure 1. Typical morphology of $CH_3NH_3PbI_3$ thin-films obtained from the 2-step method. The J-V curves indicate the typical interfacial resistance problems encountered in the given device structure are indicate by the irregular shape of the photocurrent graph.

In this work, we employ the two step-method to fabricate thin-films of the single-phase perovskite $CH_3NH_3PbI_3$, the prototype material that led to the outburst of the perovskite field. We study the growth parameters that influence the deposition process, involving the systematic study of the solvent, concentration the CH_3NH_3I solution, temperature, etc., aiming to obtain stable films at ambient conditions. Moreover, we developed alternative techniques based on this method to further improve uniformity in perovskite crystal growth. The films are characterized by X-ray diffraction, electron microscopy and optical spectroscopy to validate the quality of the films. Complete devices have been built, using the $FTO/TiO_2/m\text{-}TiO_2/CH_3NH_3PbI_3$/spiro-OMETAD/Au or $FTO/TiO_2/m\text{-}TiO_2/CH_3NH_3PbI_3$/CuSCN/Au heterojunction architecture, producing stable devices, which, however, lack charge collection efficiency (Figure 1).

The major issue encountered in the demonstration of high-performance devices so far, is the very large interfacial resistance which hampers current collection, as it is revealed from the analysis of the diode characteristics in the dark. Further device engineering designs are under examination in our lab, targeting the construction of efficient devices that will exhibit

simultaneously long-term stability and high-performance, while employing innovative approaches that can enable the fabrication of stable devices at ambient conditions.

This work was supported in part by the project “NANO-TANDEM” (MIS 5029191), co-financed by Greece and the European Regional Development Fund and in part from the Special Account for Research Funding of the University of Crete under grant numbers KA10330 and KA10652

(1) NREL efficiency chart, https://www.nrel.gov/pv/cell-efficiency.html, accessed on 24/04/2021

(2) Burschka, J., Pellet, N., Moon, SJ. *et al. Nature* **499,** 316–319 (2013)

Effect of Al_2O_3 nano composite on pure polyaniline (PANI-Al_2O_3) for tuning dielectric properties

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The present work depicts effect of Al_2O_3 nano composites on pure PANI, synthesized by in situ polymerization technique. Al_2O_3 concentration in the composites was changed from 5 to 25 wt% in the steps of 5 wt%. Structural and microstructural characterization of the synthesized composites was carried out using X-ray diffraction and scanning electron microscope. The DC conductivity was studied in the RT - 250°C temperature range while AC conductivity and dielectric behavior was studied as a function of frequency. The dielectric constant and dielectric loss were found to be change with change in the frequency values. AC conductivity of all composites was found to decrease for all frequency values which are attributed to polarization of charge carriers between the localized sites. The synthesized material may found applications in electronic devices.

Keywords: Al_2O_3; PANI; dielectric; X-ray diffraction; AC conductivity;

Formamidinium- Methylammonium Lead Iodide for Optoelectronic Applications

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In the mean of ''green energy'' and harvesting of solar radiation, solar cells predominate as the most conventional solar energy conversion devices. Many laboratories all over the world are focused on the development of the most efficient solar cell both in the power conversion as well as in the manufactory cost. Many different architectures with many different combinations of materials were developed with main goal the maximization of solar cell efficiency with simultaneous minimizing of fabrication cost.

Perovskite materials are very attractive for both high efficiency solar cells and low fabrication cost devices. The main problem that needs to be addressed, however, prior to commercialization is their sensitivity to moisture which hampers the long-term performance of the cells. For this reason, all the steps of the perovskite solar cell development need to take place in a glovebox under controllable atmosphere conditions.

In this work, we present the development of an ambient conditions process, which produces high quality perovskite thin-films with high uniformity and reproducibility. These films characterized with XRD, SEM, Uv-Vis and Photoluminescence (PL) measurements in order to investigate the film quality and morphology, the perovskite structural integrity and the films' optical properties, respectively.

We focus on double cation ($FA_xMA_{1-x}PbI_3$) solid solutions to fabricate perovskite films, judging from the fact that these systems have a better environmental stability and an energy gap close to ideal to absorb the solar radiation.

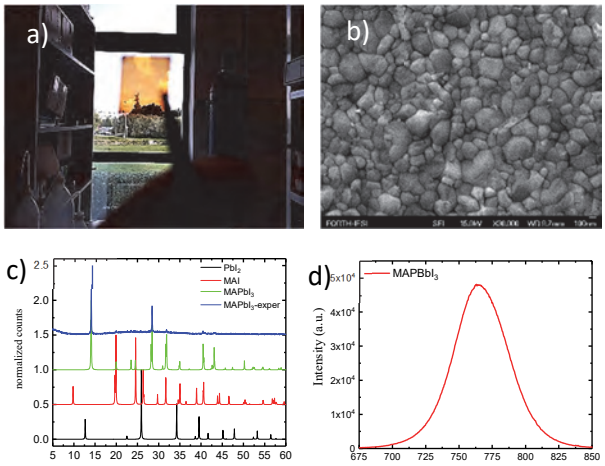

Figure 3 a) Completely uniform perovskite film, b) SEM image of perovskite structure, c) XRD pattern and c) Photoluminescence measurement of perovskite film

The complete perovskite solar cell devices were characterized with I-V measurements to extract the diode and solar cell performance. Although the film fabrication is optimized, the I-V measurements reveal a low current collection performance, which results from the high interface resistance between perovskite and transport layers and/or recombination effects on the perovskite surface. Further device engineering of these systems currently underway targets to address these issues to produce efficient perovskite solar cells at ambient conditions.

This work was supported in part by the project "NANO-TANDEM" (MIS 5029191), co-financed by Greece and the European Regional Development Fund and in part from the Special Account for Research Funding of the University of Crete under grant numbers KA10330 and KA10652 and "AENAO".

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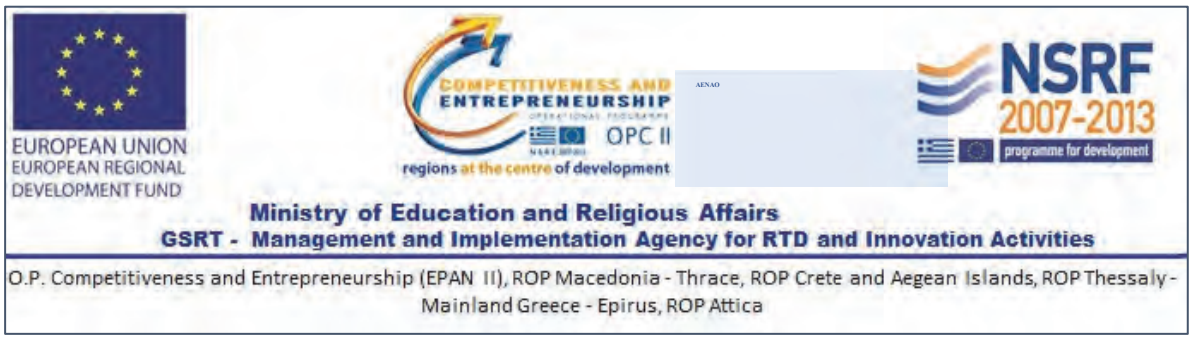

High pulsed-laser effect on the hemp composite - advanced materials

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Hemp stalk is a natural complex composite structure including cellulose, hemicellulose, lignin, pectin, wax, but also ions of calcium, magnesium, potassium and others depending on the soil composition where has grown. Pulsed laser deposition (PLD) technic performed irradiating crushed hemp stem as target with high energy laser beam led to thin layers. The materials used as supports for deposition were glass slab and hemp fabric. The analyses with FTIR and SEM-EDS spectroscopy evidenced a similar composition in the thin layer - namely Hemp Layer - as in the hemp stalk. Laser induced fluorescence (LIF) spectroscopy provided information on the fluorescent behavior of the thin layer deposited on different substrates. A coloristic method was used to analyze the composite structure of the hemp stem and of the thin layers obtained by PLD technic. Study of hemp stalk behavior under pulsed laser irradiation and use of it in the PLD technic to obtain thin films on various supports is extremely important to expanding the field of application of a plant whose cultivation brings considerable benefits to the environment both in air by the oxygen released in the process of photosynthesis and in soil by cleaning the soil and destroying pests specific to other crops. The studies carried out for this paper show an important potential for capitalization both in technical fields and advanced technologies, including optoelectronics, as well as by creating advanced materials in the field of textile technology.

Keywords: Cannabis sativa, Hemp Layer, optoelectronics, advanced textile materials

Huge ice lump fell from the atmosphere: effect of complex cumulative pollution phenomenon

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Certain human (anthropogenic) activities can produce complex phenomena in the atmosphere. Some can be useful, such as changing the weather by seeding the atmosphere at the base of the clouds with urea. In other situations, urea-based fertilizers are distributed on agricultural land in the air with agricultural utility aircraft. These sources of urea in the air, in addition to others, can at some point lead to excessive accumulation in the atmosphere. In the situation when certain favorable atmospheric conditions are met, particular and rare phenomena take place. Such an event, which took place in Targu Frumos, was investigated and is presented in this paper. Urea particles accumulated in the atmosphere from various sources of pollution, in favorable conditions of temperature, humidity and air currents, as a result of water absorption and nucleation by crystallization and freezing, formed "lumps" of ice which, reaching a certain weight fell to the ground, causing damage to a family's household. Ice samples were analyzed in FTIR spectroscopy, with urea highlighted by specific vibration bands compared to the urea control sample. The analyses were completed by UV-Vis and EDX spectroscopy, as well as by images in electron microscopy (SEM).

Keywords: urea nucleation, fertilizers, pollution

Kinetic investigation on sonochemical degradation of food dyes E132 and E127 in aqueous solution

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The sonocatalytic degradation of food dyes (E127 and E132) in aqueous solution was performed at 37 KHz using ultrasonic power of 150 W at temperature of 25 °C within 60 min, The ZnO particles were used as a catalyst to assist the sonication process. The degradation efficiency, R% of US and ZnO-H2O2-US processes were 25%, and 83.7% respectively for E127, and 15%, and 96.3% respectively for E132 after 60 min of treatment. Kinetic studies revealed that the degradation process followed the Behnajady model with the correlation coefficient $R^2 = 0.998$ for E127 and $R^2 = 0.999$ for E132, for initial dye concentration of 50 mg/L under experimental conditions. ZnO-H2O2-US process is able to remove E127 and E132.

KEYWORDS: Erythrosine, Indigotine, Sonocatalysis, Behnajady

Light interaction, pollution and SARS-Cov2: protection Mask biocompatibility-overview

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Medical protection masks or facial protection masks are briefly and insufficiently described in terms of the characteristics that must be met both in Romanian legislation and in EU directives and regulations. The recent pandemic declared in response to the alert triggered by the speed of infection with a new strain of virus, called SARS-Cov2, demonstrated the lack of specialized scientific, technical and technological documentation regarding the production of facial masks for public use to ensure effective protection against virus contamination and behavioral conditions so as not to cause adverse effects on the health of the person wearing it. Given that wearing a face mask may be also necessary in other circumstances, such as pollution itself, as well as the fact that masks are generally disposable goods eventually leading to waste generation, it is necessary to address this subject in scientific studies that can be the basis of norms and standards of materials that are effective in terms of the purpose of protection, as well as that of their destruction in safe conditions for the environment. In this context, we conducted a study on various materials to establish a hierarchy of textures of fibrous and laminated materials in terms of particle retention of 0.3 μm, this being descriptive for virus-carrying drops, as well as for various chemical compounds or dust particles that would lead to one form of contamination or another. In parallel, the impact of each type of material analyzed on the environment when it becomes waste is discussed. The biocompatibility of each of the materials is also analyzed and discussed because the mask must not only be a barrier against contaminants, but must not cause direct or indirect damage to the skin, respiration and general health conditions for the wearer.

Keywords: Standards, Virus protection, biocompatibility,

Novel $SmMnO_x$ catalyst prepared by coprecipitation coupled solvothermal for low temperature NH_3-SCR and SO_2 resistance

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A series of $SmMnO_x$ catalysts were synthesized by different methods and used for selective catalytic reduction of NO with NH_3 (NH_3-SCR). The experiment results showed that the $SmMnO_x$-CP+ST catalyst, prepared by coprecipitation coupled solvothermal method, exhibited the best low-temperature denitrification efficiency than those prepared by co-precipitation ($SmMnO_x$-CP) and solvothermal method ($SmMnO_x$-ST). More than 90% NO_x removal efficiency and N_2 selectivity were obtained on $SmMnO_x$-CP+ST catalyst in 25~200°C. Moreover, $SmMnO_x$-CP+ST catalyst showed an outstanding durability to SO_2 at low temperature. The order of SCR activity over $SmMnO_x$ was as follows, $SmMnO_x$-CP+ST>$SmMnO_x$-CP>$SmMnO_x$-ST. Based on the characterization, it was found that the superior performance of $SmMnO_x$-CP+ST could be attributed to the enhancement of specific surface area and a higher dispersion of Sm and Mn components, as well as the remarkably improved redox ability. Furthermore, the molar ratio of Mn^{4+}/Mn and (Mn^{3+}+Mn^{4+})/Mn were elevated on $SmMnO_x$-CP+ST catalyst, which played a vital role in enhancing the NH_3-SCR activity and durability to SO_2.

Keywords: NH_3-SCR; low temperature denitration; CP+ST method

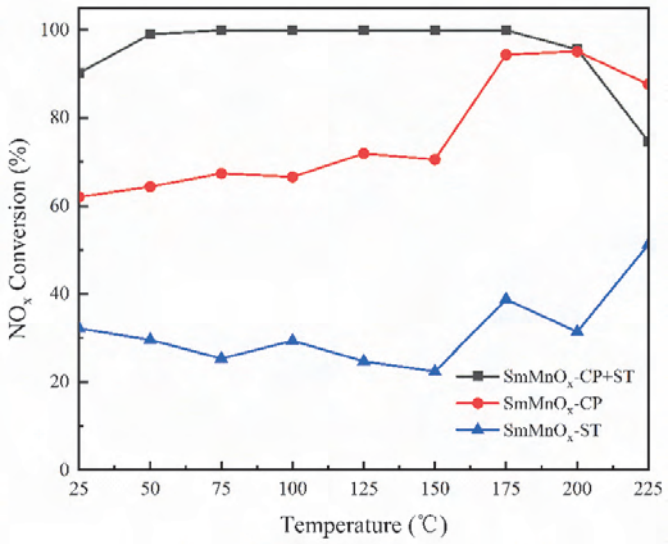

Fig. 1. The NO_x conversion of $SmMnO_x$ synthesized by different method

Magnetically separable p–n heterojunction photocatalyst SnO_2-$CuFe_2O_4$ for visible light driven degradation of azo dye methylene blue

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In the present study, p–n heterojunction $CuFe_2O_4$-SnO_2 catalyst has been prepared by two-step process; $CuFe_2O_4$ by molten salt method and facile in-situ SnO_2 composite by chemical precipitation method. The structural, morphological, and elemental analysis were conducted using Powder X-Ray Diffraction (PXRD), Scanning electron microscope (SEM), and Electron dispersive spectroscopy (EDS) to reveal the uniform distribution of nanocrystalline SnO_2 on $CuFe_2O_4$ microcrystals. Further, the composite was studied for Diffusive reflectance spectroscopy (DRS) and photoluminescence (PL) measurements to understand the bandgap engineering and charge transfer due to surface defects of the composite. The photocatalytic studies of the prepared catalyst under direct sunlight light irradiation shown 87% degradation of methylene blue azo dye, whereas the parent cubic- $CuFe_2O_4$ shown 63.5% degradation (MB). The scavenger studies and Electronic impedance spectroscopy (EIS) further elucidated the role of electrons participating in the photocatalytic mechanism and electron transfer in the composite respectively. The magnetic properties of the prepared composite were evaluated by Vibration sample magnetism (VSM) measurement. $CuFe_2O_4$-SnO_2 synthesized in the present study could be used as an efficient catalyst for the degradation of azo dyes and it is found to be magnetically separable which enhances the practical application and reusability of the composite.

Keywords: Photocatalyst; p-n hetetrojunction; Magnetic separable catalyst; Methylene blue;

Quantum Dots Pulsed Laser Deposition – a new simulation technique

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Modeling and simulation of physical and chemical phenomena has an important role in obtaining information leading to a reduction in the number of experimental trials. In this sense, for the preparation of the conditions for deposition with pulsed laser of some quantum dots of cadmium selenide (CdSe), the study of the fulfillment of the ablation conditions of the precursor materials was performed with finite element method, using COMSOL analytical software platform. Results were obtained showing the fulfillment of the ablation conditions (temperatures achieved over10^4 K) in case of using high power pulsed laser radiation applied on CdO and Se targets, as well as on CdO and Se targets, resulting in the possibility of obtaining CdSe nanoparticles and thin films, depending on how long deposition is conducted. The effect of the interaction of UV and Visible laser radiation with thin layers of CdSe deposited on the glass directly or with an intermediate thin layer was also studied. Thus, the role of depositing intermediate layers between the glass substrate and the thin layer of CdSe to reduce or amplify the response of CdSe Quantum Dots to pulsed laser irradiation by dissipating thermal energy was highlighted. The method of pulsed laser deposition (PLD) of thin layers and obtaining nanoparticles represents the prospect of developing clean, ecofriendly technologies. At the same time, the preparation of parameters and conditions through preliminary evaluations based on mathematical models and simulations reduces not only the time but also the consumption of materials and energy to set up the experiment as close as possible to the direction in which it is to be conducted.

Keywords: QDs, COMSOL, environmentally friendly, cadmium selenid

Photochemical effects on heritage asset because environmental stress

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Natural environmental factors and those generated from anthropogenic activities affect from the surface to the interior the walls of some architectural constructions leading to aesthetic distortions and later even to physical and chemical damage of the respective materials. Water is the factor with the most important contribution to such undesirable effects, especially in the conditions of a content of pollutants specific to the urban environment. In the present paper is presented the study of treatments with films of hydrophobic substances. The induced color changes are studied from the point of view of the interaction of the compounds used for hydrophobization with the material of the historical construction and as a result of the physico-chemical processes that take place under the hydrophobizing film. Colorimetric analysis is explained by changes found by FTIR and EDX spectroscopy. Images obtained with the optical microscope and electron microscope (SEM) provide information on morphological changes as a result of the modification of the sorption properties of the materials of the studied construction.

Keywords: lithic material, historical artifact, hydrophobization, colorimetry

Preparation and antibacterial performance of xanthan gum-based composite hydrogel containing green synthesized silver nanoparticles and essential oils

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Background: Silver nanoparticles are known to be effective against several healthcare-associated pathogens including antibiotic resistant ones. The antimicrobial properties of nanosilver may be exploited in the formulation of topical drug delivery systems. In this regard, hydrogels are very good vehicles/platforms/matrices that can enhance of the permeation of drugs through the keratinized epidermis.

Objective: The aim of the present study was to formulate a topical gel containing green synthesized silver nanoparticles and to evaluate the in vitro antibacterial activity of the product.

Material and Methods: Silver nanoparticles were synthesized by green synthesis, using Cinnamon extract. Xanthan gum, a gelling and thickening agent was dispersed in the silver nanosuspension. Some of the excipients (i.e essential oils) added in gel were previously dispersed in an adequate solvent before being added under constant stirring.

The presence of the silver nanoparticles was confirmed by UV-VIS analysis, revealing the fact the dimensions of the nanoparticles are approximately 30 nm.

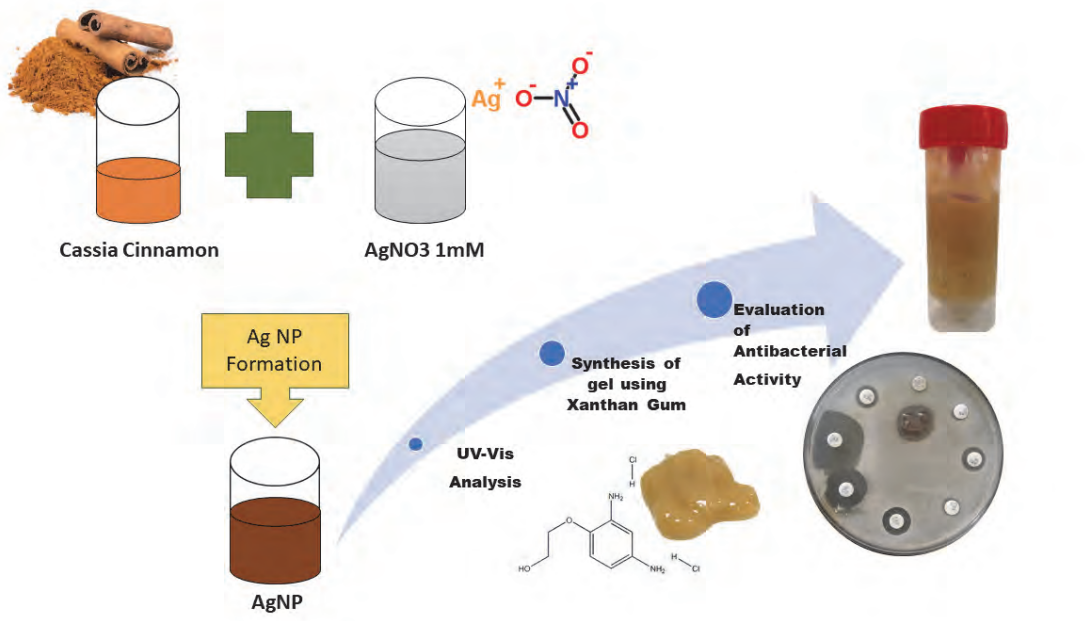
The Kirby-Bauer diffusimetric method adapted for gelling matrices was used to test the antimicrobial activity. Thus, both silver NPs dopped with *Cassia Cinnamon* and silver NPs dopped with *Cassia Cinnamon* hydrogels with essential oils were tested against Gram positive and Gram-negative bacteria. The *in vitro* antimicrobial effect of these hydrogels was assessed by the presence of the inhibition zone formed around the test sample.

Results: Results showed that the formulated gel presented a yellowish color appearance and smooth, not greasy texture, with no signs of phase separation.

The texture of the hydrogels allowed the dispersion of the active substances in the structure of the culture media and stopped the bacterial multiplication of the tested strains. The best

antimicrobial activity was identified at the silver NPs hydrogel + cinnamon apron against Gram-positive bacterial strains.

Conclusions: Overall, in the context of real-life applications of eco-friendly synthesis, this study evaluated and confirmed the in vitro antibacterial activity of a xanthan gum-based composite hydrogel containing green synthesized silver nanoparticles and essential oils.



Structural properties of copper oxide nanoparticles and their applications as photocatalysts in organic pollutants degradation

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Transition metal oxide nanostructurers have been attracted an important research attention due to their unique properties making them to find different applications in environmental protection, optoelectronics, energy storage, nanodevices or catalysis. Among various metal oxide particles, copper oxide nanoparticles have been used as photocatalysts, solar cells, gas sensors, supercapacitors, antimicrobial agents, etc. [1,2]. CuO nanoparticles were obtained by the chemical coprecipitation method which involved reacting aqueous solutions of copper precursor and sodium hydroxide as alkaline agent at room temperature, followed by calcination at 500 ^{o}C. The morphology and size of the nanoparticles were studied by scanning electron microscopy (SEM). The size of CuO nanoparticles ranges between 9-30 nm. Compositional analysis of the samples was conducted by energy dispersive X-ray analysis (EDS). The average crystallite size was estimated from X-ray diffraction (XRD) and it was found to vary in the same range above mentioned, confirming that the CuO nanoparticles present monoclinic unit cell structure. The obtained CuO nanoparticles were characterized by UV-visible absorption and Fourier transform infrared (FTIR) spectroscopy. The photocatalytic activity of CuO nanostructures was performed against Methylene Blue dye or ciprofloxacin under visible irradiation and the photoprocess was monitored examining the changes in the electronic absorption spectra. The effect of working parameters namely catalyst level and dye concentration on the photodegradation process was explored.

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Removal of methyl green from aqueous solutions by adsorption on the shrimp carapace and photodegradation using UV-C

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Effluents that are discarded by industries are important sources of water pollution because they can contain large concentrations of organic matter and have intense colour. We determine priority the influence of pH on dyes which is investigated by three different methods such as (Visual colour matching, tristimulus method, spectral method). Study has shown that methyl green is influenced by basic pH, upper 8 and demonstrated that pH affects the ADMI colour number of methyl green from aqueous solutions. We propose in this study to remove this dye by adsorption. As adsorbent, the powder shrimp carapace was used, which is low-cost, abundantly available, highly efficient, and has been reported as an alternative to the current expensive methods. Characterization of the powder shrimp carapace by chemical analysis, FTIR and SEM, was studied. Photodegradation experiments were carried out in a stirred batch photoreactor equipped with a low-pressure mercury lamp as UV source at 254 nm. The adsorption and photocatalytic experiments were conducted in a batch system at different operating parameters such as, contact time, pH, adsorbent dose, initial dye concentration and temperature. According to the experiments results, the equilibrium time, was found 112 min of contact time. Langmuir, Freundlich and Dubinin-Raduchkevich isotherm models were applied to describe the experimental data. Three simplified kinetic models were tested to investigate the adsorption mechanism. Results of the present study suggested that shrimp carapace could be suitable as a sorbent material for removal of dyes from aqueous solutions. Kinetic studies reveal that the degradation process UV-Shrimp carapace follow the The Langmuir-Hinshelwood model

Solar light driven oxidation of an organic dye with ZnO fabricated through a co-precipitation methodology

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Textile industries represent a fast-growing industrial sector, but it is well-known that such industrial activities generate highly volume of polluted effluents containing hazardous organic or inorganic compounds (such as dyes, heavy metals bleaching agents, softeners, solvents, etc). Among them, dyes represent an environmental concern because of their toxicity, bio-recalcitrance and carcinogenic feature (Khenniche et al., 2015; Rusu et al., 2014). In this context, many physico-chemical processes such as adsorption, precipitation, coagulation-floculation, membrane filtration or biodegradation were investigated or implemented for the elimination of these organic pollutants from the textile industry effluents. However, they have some drawbacks: high cost or not enough effective to treat this kind of pollution. Due to its ability to efficiently transform toxic molecules into harmless compounds (i.e. carbon dioxide, water, and mineral acids), solar photocatalysis, an advanced oxidation technique was distinguished in recent years as an outstanding green technology for the water and wastewater purification applications (Harja et al., 2020). This study focused onto the evaluation of a fabricated catalyst (ZnO powder) potential to remove hazardous water contaminants, such as organic dyes under solar driven irradiation conditions. The ZnO catalyst was synthesized through a co-precipitation method followed by a post-calcination step at 400°C. The structural, optical and morphological properties of the obtained catalyst were investigated in detail by X-ray Diffraction, FTIR analysis and Scanning Electron Microscopy. Different experiments were designed at laboratory scale mode using basic blue 41 as target molecule. For the photocatalytic performance evaluation, some investigations under batch mode and solar irradiation were conducted. Bearing in mind the optimum process conditions, the impact of some process parameters (initial solution pH, pollutant amount and catalyst load) was deeply considered. The outcomes revealed an efficient degradation of the target molecule at reaction time of 240 min at a solution pH of 6.6. Moreover, kinetic results confirmed for the basic blue 41 the Langmuir-Hinshelwood relationship (R^2= 0.996) for the initial photodegradation rates.

Summing up, the synergy between the synthesis method of the ZnO semiconductor and its photocatalytic activity under solar light develop a promising strategy for synthetic dyes removal. The performance of the photocatalytic system is attributed to the influence of process parameters (initial solution pH, catalyst load and pollutant concentration) onto the degradation

of the target molecule. These results may grant a new research key point in terms of the degradation of BB 41 dye under solar irradiation conditions, supporting the potential use of the green synthesised catalyst for perspective applications in the purification of the textile effluents.

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Synthesis and characterization of a nanophotocomposite beads based on sodium alginate and zinc oxide for wastewater treatment

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Abstract. Thanks to the specific properties that can contain hybrid materials, their application in solving environmental issues is constantly expanding from one day to the next. Therefore, their industry and manufacturing are growing very rapidly, which gives great importance to this scientific research field. Sodium alginate (NaAlg) and synthesized nanoscale zinc oxide (SNZnO) are both precursor materials used to develop these nanophotocomposite beads. These latter ones were prepared by ionotropic and chemical cross-linking extrusion method using the calcium dichloride and epichlorohydrin as cross-linkers, respectively. Several techniques were used to describe the structural, crystallographic, morphological, spectral and thermal characteristics of the prepared hybrid beads namely; X-ray diffractometry (XRD), scanning electron microscopy (SEM), attenuated total reflectance (ATR) and thermogravimetric and differential (ATG/DTG) analysis. Obtained results show a good observation of both structure and morphology of the prepared nanophotocomposite beads as well as the SNZnO was successfully immobilized in calcium alginate.

Keywords: Alginate, SNZnO, ionotropic encapsulation, chemical encapsulation, nanophotocomposite beads, characterization.

Synthesis and Characterization of Pb-free 2D Halide Perovskite Semiconductors

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Lead halide perovskites AMX3 (A+ = Cs, CH3NH3 or HC(NH2)2 , M+2 = Pb, Sn or Ge and X- = Cl, Br or I) have taken the semiconductor field by storm in the last decade, guided by the immense development of efficient photovoltaics that have reached power-conversion efficiencies >25%. A notable class among them is dimensionally reduced two-dimensional (2D) perovskites that offer much greater sensitivity to moisture and boost the devices' performance through stable excitonic features at room temperature. However, in most of the materials the prevailing semiconducting properties derive from the presence of Pb, which is renowned for its high toxicity. Because of this, Pb-free perovskite compositions have been actively explored in the past five years. Lead-free compositions have demonstrated a variety of interesting physical qualities which in combination with their low toxicity make them an alternative direction towards the discovery of novel inorganic semiconductors. The most chemically sensible candidate metals to substitute for Pb in the Pb-free class belong in the group 14 metal family as well as in the expanded double perovskite classes (1).

In this work, we demonstrate that 2D, Pb-free perovskites based on Ge and mixed metal Ag-In compositions can be obtained using low-temperature wet chemistry. The new compounds, which possess the Ruddlesden-Popper structure-type, have been characterized by single-crystal and powder X-ray diffraction and their optical properties at room temperature were determined (Figure 1). The compounds possess a strong optical absorption in the visible likely deriving from a direct band gap transition. These features render the Ag-In and Ge based 2D hybrid perovskites promising lead-free perovskite families, suitable for integration into optoelectronic devices, exhibiting superb environmental stability. Understanding the structural features of these emerging, "green" perovskites and understanding their underlying physical properties will pave the way for a new generation for environmentally-friendly, efficient optoelectronic devices.

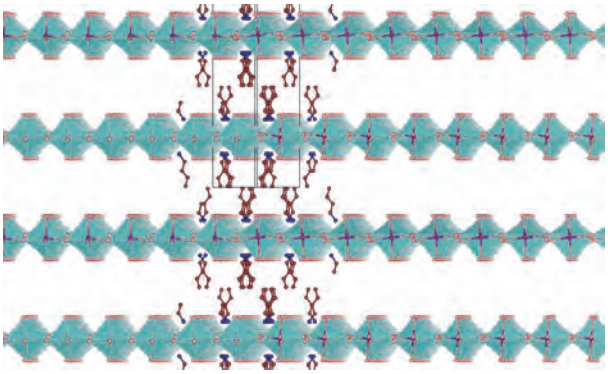

Figure 4: Typical layer stacking of a hybrid 2D perovskite based on Ge. The shaded polyhedral consist of $(GeI_{6/2})^-$ octahedra whereas the organic cations interdigitate between the two-dimensional sheets.

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Washing municipal streets – the origin of some photo-contaminants pollution

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This paper is an environmental investigation under conditions of anthropogenic pollution resulting from operations intended to reduce pollution and which prove not only ineffective, but which add more pollution when applied improperly. The use of so-called "dust-binders" to produce the coagulation / flocculation of dust particles, but also of organic compounds in urban areas, on the streets without being followed by vacuum cleaning, leads to episodes of pollution. Washing the streets in such situations only disperses polluting compounds into the environment in the immediate vicinity. The analysis of the street washing water and the resulting foam showed in the FTIR and EDX spectroscopy the presence of coagulating / flocculating compounds based on aluminum (aluminates and derivatives), as well as anti-skid (calcium chloride), together with the bound compounds, namely dust particles and organic compounds. By scanning electron microscopy (SEM), the agglomeration structures were highlighted as a result of the coagulation / flocculation processes. The results of the study in this paper indicate the need to develop a methodology and rules for the use of coagulants and anti-skid so as to protect the environment from an additional supply of pollutants.

Keywords: dust-binders, aluminate, anti-skid, coagulants/flocculants, cleaning induced water contamination process

White-light emitting layered hybrid lead halide perovskites

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Semiconductors have formed the basis of a revolution in technology and are prevalent in all sectors of our economy including power generation, transportation, communications, and health care. They play a key role in clean energy by employing clean, renewable energy sources and improving energy efficiency. Among them, the emerging class of halide perovskites stands out of the field, given that within only few years they have been able to leapfrog many long-researched materials. Halide perovskites are remarkable semiconductors as they have high optical absorption coefficients, long charge carrier diffusion lengths, intense photoluminescence, and slow rates of non-radiative charge recombination. Recent years have seen another iteration in the development of the materials with the emergence of two dimensional variations of the perovskite structure. Layered hybrid halide perovskites ($A^{I}_2B^{II}X_4$ or $A^{II}B^{II}X_4$ (A=monovalent or bivalent cation), B=bivalent p-block metal, Pb, Sn or Ge), X=halide anion, Cl, Br or I), consist of anionic sheets of corner-sharing metal-halide octahedra, selectively "partitioned" by organic cations to form crystallographically ordered nanoscale sheets. This arrangement generates natural multiple quantum wells that exhibit stable excitonic features with intense photoluminescensce (PL) characteristics, even at room temperature. Some of the materials exhibit unusual optical emission, since they can generate white light as a result of the self-trapped exciton mechanism (1). The generation of white light by a single material has great implication for solid-state lighting applications, especially since the produced white light emission affords tunable color rendering and high quantum efficiency.

In this work, we will present the synthesis and optical characterization of two layered amide halide perovskites*: $(GABA)_2PbBr_4$* (GABA = γ-Aminobutyric Acid), *$(HIS)PbBr_4$* (HIS = histammonium) and their derivative structures. The compounds have been crystallographically and spectroscopically characterized revealing a high phase purity and an intense PL emission (Figure1).

The selected two-dimensional hybrid perovskites exhibit an optical emission, centered around 2.5 eV despite having a bandgap at $E_g \sim 3$eV. The understanding of the emission mechanism of these material with respect to the structural properties of the perovskites will allow us to fine-tune the white-light emission, which will optimize these materials for solid-state lighting applications and energy saving devices.

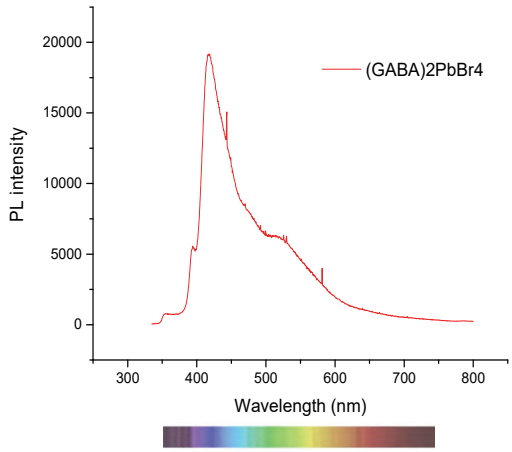

Figure 1. PL spectrum of $GABA_2PbBr_4$ at room temperature with λ_{exc} = 325nm.

CCS acknowledges support from the Special Account for Research Funding of the University of Crete under grant numbers KA10330 and KA10652.

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