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ABSTRACT BOOK

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Plenary Talks

Circular Upcycling of Electronic, Industrial, and Coal Waste into High-Performance Catalysts

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Abstract

The rapid growth of electronic devices, industrial manufacturing, and energy production has led to unprecedented accumulation of complex solid waste, posing environmental risks while simultaneously containing valuable elemental and mineral resources. Developing scalable routes that transform such heterogeneous waste into functional materials is thus central to sustainable materials engineering and circular economy strategies. Here, we present an integrated waste-to-function platform that converts three abundant and difficult-to-manage waste streams, spent Ni–MH batteries, industrial titanium scrap with fallen leaves, and pond coal ash, into high-performance catalytic materials for energy and environmental applications.

From spent Ni–MH batteries and aluminium foil waste[1], we recovered $NiSO_4 \cdot xH_2O$ and Al precursors, and synthesized Ni $(OH)_2$ hydrogel-derived Ni/η-Al_2O_3 nanocatalysts with 4% and 8% Ni loading. The 8% Ni material exhibited outstanding CO_2 methanation performance, achieving 99.8% CH_4 selectivity and a space time yield of 80.3 mmol CH_4 g_{cat}^{-1} h^{-1} at 400 °C. *Operando* DRIFTS coupled with GC and MS revealed an associative methanation pathway *via* hydrogenated carbonate, formate, and methoxy intermediates[1].

Using industrial Ti scrap and fallen leaves[2], we produced P-, N-, and C-doped TiO_2 nanoparticles using a fully waste-derived synthesis route. The dopants stabilized anatase against rutile conversion even after calcination at 700 °C, suppressed electron hole recombination by a factor of 7.3 compared to commercial P25, and enabled about 96% sunlight-driven removal of surface adsorbed pollutants when incorporated into water-based polymeric paints without degrading the polymer binder, as confirmed by micro-FTIR surface analysis[2].

Finally, pond coal ash collected from power plants in Mongolia was fractionated by wet magnetic separation into magnetic and non-magnetic streams and upcycled into low-cost CO oxidation catalysts[3]. The non-magnetic fraction consistently outperformed the magnetic one, delivering about 44% higher CO conversion at 400 °C and about 31% higher conversion at 450 °C. Across all three case studies, comprehensive structural, surface, and *operando* analyses

demonstrate that catalytic performance is governed by mineralogical complexity, surface heterogeneity, and redox flexibility rather than elemental abundance alone.

Overall, these examples demonstrate the transformation of hazardous, low-value waste into sustainable catalysts. By enabling greenhouse gas conversion, air purification, and self-cleaning surfaces, this work advances circular materials chemistry toward viable environmental technologies.

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Beautiful Defects: Designed Thin Films for Sustainable Performance

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Abstract

Defects are traditionally considered imperfections that limit material performance and reliability. Recent advances in thin-film research demonstrate, however, that interfaces, stacking faults, local chemical fluctuations, and metastable phase boundaries can be deliberately designed to enable superior and sustainable functionality.

This plenary lecture highlights how defect engineering in vapor-phase deposited nitride, carbide, boride, and oxide thin films governs key performance metrics, including hardness, fracture resistance, thermal stability, and resistance against oxidation, irradiation, and hydrogen permeation. Particular emphasis is placed on nanostructured and compositionally complex thin films, where the interplay between chemical disorder, elastic strain, and phase stability gives rise to emergent properties unattainable in conventional materials.

Beyond materials performance, the lecture addresses technological aspects that are critical for sustainable manufacturing. The use of powder-metallurgically prepared alloyed sputtering targets enables sputter-yield amplification effects, leading to massively increased deposition rates without compromising coating quality. Carefully selected heavy and reactive alloying elements and secondary phases modify collision cascades and secondary electron emission, allowing dense coating architectures to be achieved at significantly reduced substrate and chamber heating. Complementary plasma control strategies further enable dense microstructures while minimizing thermal load.

By combining advanced thin-film synthesis, state-of-the-art characterization, and density functional theory, a mechanistic understanding emerges of how “beautiful defects” simultaneously enhance material performance and process efficiency. The talk concludes by illustrating how defect-by-design approaches reduce processing time, energy consumption, and CO2 footprint, thereby contributing to resource-efficient and economically viable materials solutions for energy, mobility, and extreme-environment applications.

Keynote Talks

Magneto-Plasmonic Nanodevices for Nanotherapies, Green Synthesis and Water Remediation

Aritz Lafuente[1], Arnau Fons[1], Mar Álvarez[1], Albert Serra[2], Elvira Gómez[2], Alejandro Gómez-Roca[3], Maria José Esplandiu[3], Josep Nogues[3] and Borja Sepúlveda[1]*

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Abstract

There is a critical need to develop new cost-effective micro/nano materials and devices to help in the transition towards a more sustainable and green economy. Here we present our latest developments in photo-thermal and photo-electric catalytic micro/nanodevices for nanotherapies, energy and environmental remediation.

In the biomedical field, we will present magneto-plasmonic nanocapsules (MAPSULES) for wirelessly controlled drug delivery, bioimaging and nanothermometry [1, 2]. The MAPSULES endow unprecedented magnetic strength, colloidal stability, photothermal efficiency and biodegradability. By exploiting the magnetic and optical control, we have demonstrated complete tumor ablation at ultralow drug concentration (i.e., between 200 and 500-fold lower than the therapeutic window of the free drug). This versatile technology can also be applied to photothermal and photodynamic therapies, anti-bacterial treatments or nanothermometry.

In the case of energy, we have developed magneto-plasmonic nanosystems that efficiently harvest light to generate photo-thermo-catalytic reactions. In particular, we will present Ni-based nanocatalysts exhibiting intense broadband optical absorption for the photothermal synthesis of the high added-value biofuel precursor gamma-valerolactone from biomass residues [3]. This catalytic strategy enables remarkable reduction of reaction temperature and time, thereby opening paths towards industrial applications.

In environmental remediation, we will show how magneto-plasmonic catalysts can be integrated within photo-electric devices to generate controlled catalytic redox reactions [4]. We exploit this to achieve a highly amplified mineralization of organic pollutants under low light intensities (5-fold lower than sunlight). Moreover, we have developed the novel concept of pulsed photo-electrochemical actuation to enhanced even further the reaction kinetics and reducing, simultaneously, the required light input power [5].

In conclusion, magneto-plasmonic nanodevices represent a promising frontier in materials science/engineering. By harnessing the synergistic optical and magnetic effects, these

systems have the potential to address critical challenges in energy, and environmental remediation.

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Graphene Mesosponse for Energy Applications

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Abstract

Although graphene-based materials with three-dimensional (3D) framework are expected for scalable energy applications, most materials reported thus far have encountered issues in precisely controlling graphene stacking, excluding graphene edge sites, and controlling nanoporous structures. This presentation will highlight a novel 3D graphene material, customized for fast and durable energy storage, called Graphene MesoSponge (GMS: *Adv. Funct. Mater*, **26**, 6418-6427 (2016)).

GMS is synthesized by a hard-templating method using nanostructured metal oxides, such as Al_2O_3, MgO, or SiO_2, *via* precisely controlled chemical vapor deposition in which the average stacking number of graphene sheets is adjusted to approximately 1. After template removal under appropriate conditions in which the framework is well retained, the resulting mesoporous carbon is subjected to thermal treatment between 1600 to 1800 °C to eliminate graphene edge sites *via* zipping reactions. Thus, GMS exhibits ultra-high stability against chemical and electrochemical oxidation. Despite such durability, GMS possesses a high surface area (ca. 2000 m^2/g) and a large pore volume (> 3 cm^3/g). Moreover, GMS has a high electric conductivity superior to carbon blacks. Furthermore, GMS has sponge-like flexibility and mechanical toughness. Such unique properties of GMS enable its use as next-generation durable and high-performance carbon material for battery-related applications. As an electrode material for electric double-layer capacitors, GMS exhibits ultra-high voltage stability up to 4.4 V even in a conventional organic electrolyte (Et_3MeN/BF_4), which surpasses single-walled carbon nanotubes. Moreover, its mesopores can facilitate fast ion transfer, and the rate performance can be further improved by fabricating nanoplate-shaped GMS particles. Also, GMS fulfills conflicting requirements for a cathode of lithium-oxygen batteries. Not only showing extremely high capacity (6700 mAh/g), we found that the topological-defect-rich structure exhibits unique catalytic properties to form easily decomposable nanosheets of Li_2O_2, leading to a low charge plateau (~3.6 V (vs. Li/Li^+)). With its unique edge-site-free and topological-defect-rich structure, GMS achieves a record cycle performance (307 cycles, > 1535 h). Furthermore, its performance can be significantly improved by creating a self-supported GMS sheet with tunable porosity, specific surface area, and thickness to achieve unparalleled performance in terms of capacity, rate performance, and cyclability.

Hydrogen Production from Positive Electrode Materials in Lithium Ion Rechargeable Batteries due to Water Splitting

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Abstract

The production of hydrogen molecules (H_2) by splitting water (H_2O), which is a renewable resource, using electrolysis, photo-catalysis, solar energy, and other such methods, is one of the most attractive processes, involving zero emission of carbon dioxide (CO_2). It is important to split H_2O at low temperatures and electric powers and, in addition, to store and release significant amounts of the produced H_2 by spending minimal energy in order to reduce the cost of this H_2 production process.

The aim of this work was to investigate the H absorption and desorption characteristics of Li_xCoO_2 (x=1.00, 0.75, 0.50) positive electrode materials in lithium ion (Li^+) rechargeable batteries, soaked in H_2O at room temperature. Thus, the H concentration of $LiCoO_2$ materials exhibiting H_2O-uptake was investigated in air using weight gain (WG) measurement and ion beam surface analysis, which was combined with high-energy elastic recoil detection (ERD) with 16 MeV O^{5+} and 5.1 MeV He^{2+} ion-probe beams. In addition, the release of hydrogen molecules (H_2) and the dissociation temperature were characterized using gas chromatography (GC). In addition, first-principles calculations performed using a density functional theory (DFT) code were also examined to elucidate the most stable sites for trapping H in $LiCoO_2$ after H_2O uptake.

In the present study, the results by WG, ERD, GC, and DFT revealed that the release of H_2 was clearly confirmed by heating the H_2O-soaked $LiCoO_2$ up to the lower temperatures less than 523 K and, in addition, the production of H_2 might occur owing to the desorption of H atoms from the Li substitutional sites and the recombination of activated H atoms. These results suggest a potential new application of spent Li-ion batteries for H storage by H_2O splitting at room temperature.

Invited Talks

Zero-Field Superconducting Diode Effect in Artificial Multilayers

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Abstract

The diode effect is fundamental to modern electronics, playing a key role in rectification and AC–DC conversion. However, at low temperatures, conventional semiconductor diodes exhibit large resistance, leading to increased energy dissipation and undesirable heating during operation.

Recently, various phenomena, including the superconducting diode effects (SDEs), have been observed in noncentrosymmetric superconductors1, 2. In particular, recent experiments have demonstrated the zero-field SDE, wherein the superconducting current flows only in the forward direction3-5, as shown in Fig. 1. Incorporating ferromagnetic layers and an asymmetric stacking structure breaks time reversal and space inversion symmetries, enabling the observation of nonreciprocal responses such as the zero-field SDE. Specifically, the polarity of the SDE could be manipulated by adjusting the magnetization direction of the ferromagnetic layers. These results indicate that the proximity effect at the superconductor/ferromagnet interface can be used to effectively control the SDE. Zero-field SDEs have the potential to enable novel nonvolatile memory devices and logic circuits with ultralow power consumption owing to their similarity to semiconductor diodes.

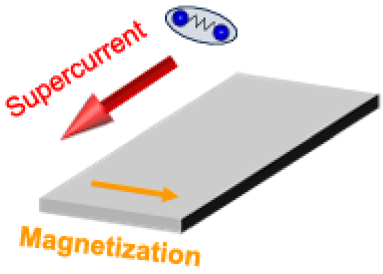

Fig. 1 Zero-field superconducting diode effect

In this presentation, I discuss the magnetization control of zero-field SDE in asymmetric artificial multilayers without time-reversal and space-inversion symmetries. In the ferromagnetic polar multilayers, these symmetries are broken due to magnetization and an asymmetric structure, leading to the zero-field SDE. Additionally, multilayers stacked at the nanoscale behave as a single new superconductor across the entire multilayer structure. For example, when the magnetization directions of the ferromagnetic layers above and below the superconducting layer are parallel, the nonreciprocal critical current becomes finite. In

contrast, the nonreciprocal critical current vanishes for antiparallel magnetization configurations. This characteristic enables the control of the zero-field SDE, allowing polarity reversal and ON/OFF switching.

The proposed symmetry-breaking process using an artificial stacking structure is highly versatile. Additionally, periodic ferromagnetic insertion enables tuning of the superconducting transition temperature and control of the nonreciprocal critical current. In nanoscale multilayers, even when the volume fraction of ferromagnetic material is kept constant, variations in ferromagnetic layer thickness, the number of insertion points, and their spatial arrangement exert diverse effects on superconductivity.

Furthermore, artificial multilayers offer additional flexibility for engineering electronic band structures through the choice of elements, layering sequence, film thickness, and periodicity, making them a promising platform for exploring new superconductors with practical functionalities. The results of this study can contribute to the development of rewritable superconducting-diode logic circuits by exploiting the nonvolatility of magnetic materials.

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When the Surface is the Device: Hints from DFT Calculations

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Abstract

This paper aims at showing how first-principle simulations based on the Density Functional Theory (DFT) can provide very relevant hints on the design of functional interfaces for applications in various fields related to the design of new materials for energy and the environment. Indeed, the functionalization of surfaces with molecules or nanometric particles is often the key to tune the properties of a material. However, a reliable description at the atomic level of the interfacial region, though crucial, can be hard to achieve experimentally. Here, it will be shown how DFT simulations, in close contact with advanced surface science experimental techniques such as STM, XPS, and HREELS, contribute to the deep understanding of the chemical and physical properties of surfaces.

The first part of the talk deals with the bonding of N-heterocyclic carbenic and olefinic molecules on metal and metal oxide surfaces. The interplay between steric and electronic structure of the molecule, on the one hand, and the surface, on the other, dictates the stability and mobility of the grafted species. On copper surfaces, various diffusion mechanisms are presented, to explain the aggregation of the molecules in ribbons and islands. A computationally assisted assignment of some selected vibrational modes is used to depict the binding mode and the molecular orientation on the surface. On reducible metal oxides, notably, the carbene molecules are found to bind strongly to oxygen atoms, at variance to what commonly observed in organometallic coordination chemistry. On non-reducible oxides, a carbon-metal cation bond is observed. The implication of this tunable bonding mode in creating functional structures and new materials is discussed.

Next, a computational study of transition metal nanometric and subnanometric clusters on MgO thin films supported on Ag, and 2D-MXenes is presented. The interaction with the support is shown to dictate the charge state of the supported nanoclusters. The relevance of the metal-support interaction is unveiled by looking how oxygen species can diffuse on supported Ni. Pd, Pt clusters, changing their charge state and enhancing their binding to the support. The activation of key-molecules for green chemistry such as CO_2 and CH_4 is then discussed, with particular emphasis to the role of the support.

Confined Crystallization in PEDOT: PSS: Tailoring Charge and Heat Transport for Thermoelectric Energy Harvesting

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Abstract

Thermoelectric materials provide a solid-state route to energy conversion by directly transforming temperature gradients into electrical power. Their performance is governed by the Seebeck coefficient (S) which should high to efficiently convert heat into voltage, the electrical conductivity (σ), which should be high to ensure effective charge transport and the thermal conductivity (k), which should be low to maintain a temperature gradient within the material.

Organic thermoelectric materials are particularly appealing in this context. They are generally expected to exhibit relatively low k and, at the same time, offer several advantages as green functional materials, including metal-free composition, mechanical flexibility and compatibility with low-temperature, solution based processing on flexible and large-area substrates. Nevertheless, their use is still hampered by a reduced figure of merit, *zT*, largely associated with limited electrical conductivity and with the difficulty of optimizing all thermoelectric parameters at the same time.

In this contribution, I will present a material–process strategy that exploits crystallization in confined environments to tune charge and heat transport in conducting polymers, using PEDOT: PSS as a benchmark system. By controlling film formation through a lithography-controlled wetting technique, we first prepare patterned films with ≈850 nm-wide stripes at the surface that show improved crystallinity and PEDOT chain packing compared to spin-coated counterparts. Under these conditions, σ is strongly enhanced, while the in-plane thermal conductivity (k‖) increases only marginally, leading to a maximum power factor of 201 µW m^{-1} K^{-2} and a *zT* enhancement in the 110–260% range with respect to spin-coated films. [1]

We then push confinement further, promoting the formation of ≈150 nm-wide stripes. At this length scale, the narrow conducting features enhance phonon–boundary scattering, resulting in a reduction of k‖ by up to 30% compared to spin-coated films. For these more confined films subjected to secondary doping, S is also found to slightly increase relative to equally treated spin-coated samples, consistent with the additional narrowing of the conducting domains and with a transport regime approaching one-dimensionality.

Altogether, crystallization of PEDOT:PSS in confined environments leads to concurrent improvement of σ and S together with a significant reduction of $k_\parallel$, effectively relaxing the conventional correlations among thermoelectric parameters and yielding power factors up to ~300 μW m^{-1} K^{-2} with a marked increase in *zT*.

This material–process strategy offers a simple, scalable route to engineer metal-free, solution-processed conducting polymers for thermoelectric energy conversion and, more broadly, for functional green electronic materials.

Modulation of Transition Metal Dichalcogenides *via* Interface Engineering with Molecules and Polymers

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Abstract

Transition metal dichalcogenides (TMDCs) have attracted significant attention as device materials and as platforms for materials science and physics, owing to their unique atomically thin layered structure. One important research direction is their use as channel materials in advanced field-effect transistors. Although TMDCs have enabled narrow-channel devices and demonstrated 3D-stacked architectures, significant challenges remain in modulating carrier concentrations and controlling contact resistance to fully use their performance. In this talk, I will present our recent work on modulating the electronic states of TMDCs through interface engineering with molecules and organic polymers, achieving substantial modulation from the conventional semiconducting state to metallic and semi-metallic states. Furthermore, our studies have enabled the assembly of thin organic layers on TMDCs, creating opportunities for integration into device architectures.

Nowadays, monolayer TMDCs can be readily prepared on substrates, which enables efficient analysis of their chemical modifications and properties. We have developed a method to modulate carrier concentrations in MoS_2, converting it from a semiconducting to a metallic state. By interfacing TMDCs with organic materials, we induced electron transfer at the interface, which resulted in metallic behavior. Specifically, I will present examples involving redox-active molecules [ref.1] and non-redox-active molecules [ref.2] to efficiently tune these properties.

The second topic addresses phase modulation of MoS_2 to induce a semi-metallic state. We developed a gentle oxidation combined with polymer encapsulation, enabling phase transformation from the semiconducting 1H phase to the semi-metallic, topologically protected 1T′ phase [ref.3]. This approach further allows the formation of lateral junctions and vertical heterostructures (1T′ on 1H). These features hold promise for creating metallic contacts and reducing contact resistance in future device applications.

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Synthesis of Al-5Mg (wt %) Alloy *via* Powder Metallurgy Route using Hot Pressing

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Abstract

Mechanically alloyed powders were hot pressed to synthesize Al-5Mg (wt%) alloy, with an emphasis on the effect of holding time during hot pressing on densification, microstructure, and hardness of the alloy was studied, hot pressing was conducted at a temperature of 550 °C under constant pressure of 45 MPa, using holding times of 30, 60, and 90 minutes. The consolidated samples were characterized in terms of density, microstructural evolution, and hardness. Density was measured to evaluate the extent of densification achieved at different holding times, while optical microscopy and scanning electron microscopy (SEM) were employed to examine grain morphology, phase distribution, and porosity. Vickers hardness testing was conducted to assess the mechanical response of the hot-pressed bulk consolidated sample. Corrosion behaviour of the alloy has been carried out using potentio dynamic studies. The results demonstrate that increasing the holding time during hot pressing significantly influences densification and microstructural uniformity with relative densities of 85.5%, 89% and 95% for 30, 60, and 90 minutes, which in turn exhibits the improved hardness values of 98 HV, 112 HV and 120 HV of the alloy, respectively.

Ultra-Small Metal/Ionic Liquid Interfaces on Layered Niobates for Hydrogen Production *via* Methanol Photoreforming.

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Abstract

This study presents a fast and eco-friendly strategy to develop a photocatalytic system based on potassium hexaniobate ($K_4Nb_6O_{17}{\cdot}xH_2O$) modified with sub-nanometric copper clusters (SNCu) produced *via* sputtering. With a low metal loading (less than 1%), the material shows excellent hydrogen production from methanol photoreforming (MPR) and water splitting reaction (WSR) under simulated sunlight. Encapsulation with an ionic liquid [BMIm] [NTf_2] leds to the system (IL@SNCu@KNbO) enhancing activity and stability, reaching 170 µmol H_2 (4,000 $\mu mol{\cdot}g^{-1}{\cdot}h^{-1}$; AQY = 26.8%) and outperforming SNCu@KNbO (160 µmol) and pristine KNbO (2.9 µmol). Structural and spectroscopic analyses confirm homogeneous SNCu dispersion and strong metal-semiconductor interactions. The IL plays a key role in improving interfacial charge dynamics, forming a polar nanolayer that modifies the band gap (from 3.64 to 3.81 eV), broadens the valence band, and suppresses photoluminescence by ≈ 80% which is an evidence of reduced recombination. XPS and solid-state NMR demonstrate that the IL remains chemically stable, protecting SNCu sites against aggregation and photo-corrosion. Replicate experiments show that while the IL significantly enhances pristine KNbO, its effect is partially masked in SNCu@KNbO due to the strong electron-sink behavior of the ultra-small copper clusters. Stability tests reveal consistent performance over four cycles, with moderate activity loss after the sixth cycle associated with 0.84 ppm Cu in solution and TGA indications of partial IL restructuring. The catalyst remains functional and durable by four cycles, demonstrating the potential of combining sputtered SNCu clusters with IL encapsulation as a sustainable route for hydrogen generation using low metal loadings and environmentally friendly processing.

Porous Carbon Pellets from Cellulose Acetate for High-Volumetric Hydrogen Storage

Hiroshi Matsutaka[1, 2]*, Aya Kashifuku[1], Takaaki Orii[1], Daigo Miyajima[1,3], Naoki Uchiyama[1,4], Satoshi Wada[1], Hirotomo Nishihara[2,5]

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Abstract:

Material-based hydrogen adsorbents, such as activated carbons and metal-organic frameworks (MOFs), are promising for hydrogen energy storage, providing safer and more efficient alternatives to high-pressure gas tanks. Although some MOFs have recently achieved very high specific surface areas per unit weight, their low bulk density limits their volumetric storage capacity. Increasing density through molecular design or compression often results in the loss of pore structure. One key approach is pelletizing techniques that maintain adsorption performance while improving volumetric storage density. This study focuses on cellulose acetate-derived porous carbons, which are known to be applicable as volumetric high-hydrogen adsorbents. By adjusting the KOH activation conditions after hydrothermal synthesis of the cellulose acetate and then applying high-pressure compression (800 MPa), porous carbon pellets were produced. These pellets achieved a high bulk density without significantly damaging the pore structure, resulting in improved volumetric hydrogen storage performance (20 g-H_2/L at -196°C and 1 bar). This approach demonstrates a viable pathway for producing volumetric high-density hydrogen adsorbents. (Ref.) Hiroshi Matsutaka *et al.*, *J. Mater. Chem. A*, **13**, 22392-22405 (2025)

Plenary Talk

Redox Aspects of Lithium Ion Batteries

Hubert Girault*

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Abstract

The lecture will address the redox aspects of electrical batteries, with a particular emphasis on lithium-ion systems. We will revisit several fundamental notions, including the concept of the Fermi level of electrons in solutions, the notions of capacitance and pseudo-capacitance, and some basic terminology and definitions that have often been misused in the battery field.

We will examine the fundamental mechanisms of intercalation reactions in redox-active particles such as metal oxides and metal phosphates, where electroneutrality is maintained through the intercalation of cations such as Li^+. We will also discuss the electrostatic intercalation of lithium cations into graphite, along with the precipitation of the various staged phases, including LiC_{12} and LiC_6.

In conclusion, we will show that a so-called lithium-ion battery employing a graphite anode is in fact a mixed electrochemical storage device: it combines redox-active solid particles at the positive electrode with a volumetric graphite capacitor at the negative electrode.

Keynote Talks

Green Methods for the Synthesis of Phosphinates, Phosphonates and Tertiary Phosphine Oxides

György Keglevich

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Abstract

During our purpose to synthesize the title compounds as intermediates or potentially biologically active agents, we applied green methods.

The different P-esters are usually prepared from the corresponding P-chlorides. Going green, phosphinates, alkylphosphonates and dialkoxy-phosphates were synthesized by the microwave (MW)-assisted direct esterification of phosphinic acid, phosphonic acid and alkoxyphosphonic acid, respectively, applying alcohol as the reactant. Suitable ionic liquids as catalysts promoted the estererifications [1–3]. In the above case, MW irradiation made possible otherwise thermally impossible transformations.

Next, we aimed at syntheses, where MW irradiation substituted the cost meaning and environ-burdening catalysts. Such reactions are the tree-component Kabachnik–Fields condensations of oxo-compounds, primary or secondary amines and dialkyl phosphites to afford α-aminophosphonates [4]. Tandem phospha-Mannich reactions were also elaborated [5], and the aminophosphonates were modified [6].

In the following typical case, MW irradiation allowed the simplification of the catalyst system. A good example is the Hirao P–C cross-coupling reaction of bromoarenes and >P(O)H reagents including secondary phosphine oxides to furnish arylphosphonates or tertiary phosphine oxides [7]. In these cases, the excess of the P-reagent substituted the traditional mono- and bidentate P-ligands *via* their trivalent tautomeric form (>P-OH) needed in the Pd-complex catalyst. Ni-complexes could also be applied in a similar way [8]. Moreover, potentially cytotoxic derivatives were also prepared [9].

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Cellulose-Based Hierarchical Structures: Linking Chirality and Functionality in Green Materials

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Abstract

Cellulose, a chiral polymer abundantly produced by plants, forms hierarchical helicoidal structures across multiple length scales. These architectures govern structural colouration, mechanical strength, and environmentally responsive motion. Chirality appears from the molecular to the macroscopic scale—seen in plant tendrils with alternating twists [1] and in Erodium seed awns and Pollia condensata fruits showing right-handed and nanoscale chiral structures [2].

Inspired by these natural systems, this work investigates the existence of left- and right-handed twisted structures in thermotropic cellulose derivatives at room temperature [3]. Free-standing cholesteric films contain distinct left (LH) and right-handed (RH) structures whose pitches respond oppositely to strain—LH expands while RH contracts—due to differently oriented optical axes. When overstretched, the films spontaneously recover their shape within minutes, accompanied by reversible shifts in circular dichroism of the chiral pitch. These results reveal a dynamic, strainresponsive hierarchical organization in solvent-free cellulose liquid crystals.

Acknowledgments

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Experimental Journey at the Edge of Quantum Materials

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Abstract

Over the last decades, condensed matter physics has been the playground for the realization of physical systems in which quantum effects persist over a wide range of energy and length scales [1]. The resulting quantum materials include topological insulators, topological crystalline insulators, magnetically doped topological quantum materials, 2-dimensional van der Waals (2D vdW) materials, Kitaev- , and spin-orbit-materials, *etc…* [2].

An overview is here given on the most relevant research results we have achieved on emergent phenomena in quantum materials, with particular attention to topology, symmetry, and spin-orbit coupling. The summary overarches the demonstration of Rashba spin-orbit coupling in wurtzite *n*-GaN:Si [3,4], the discovery of infra-red optically active centres in (Ga,Mn)N:Mg, the electronic characteristics that emerge in the Mn doped topological crystalline insulator SnTe [5] and in the intrinsic ferromagnetic topological insulator $Mn(Sb,Bi)_2Te_4$. Moreover, it is shown that the study of 2D topological semimetals has revealed (i) quantum chiral anomaly in flakes of the Weyl semimetal T_d-WTe_2 up to a record temperature of 100 K [6], and (ii) Pt vacancy-induced Kondo effect in non-magnetic $PtSe_2$ [7,8].

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Green design of Biopolymer Hydrogels for Regenerative Wound Care: Evidence from *In-vivo* Study

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Abstract

Delayed wound healing, particularly in diabetic conditions, represents a serious clinical and socioeconomic burden due to persistent inflammation, oxidative imbalance, and insufficient tissue regeneration. Natural polymer-based hydrogels have recently attracted considerable attention as modern wound dressing materials because they can maintain a moist microenvironment, support cell growth, and serve as carriers for therapeutic agents. At the same time, integrating plant-derived compounds into biomaterials offers opportunities to apply sustainable and circular economy principles by utilizing agro-industrial byproducts.

In this work, a biodegradable hydrogel formulated from alginate and gelatin and supplemented with grape skin extract was investigated as a regenerative dressing in an *in vivo* diabetic wound model. Grape skins, a residual material generated during wine production, contain high levels of polyphenolic compounds known for their antioxidant and anti-inflammatory activities. Their incorporation into hydrogel systems enables the valorization of waste materials while providing biologically active molecules beneficial for tissue repair. The healing potential of the developed hydrogel was examined in streptozotocin-induced diabetic rats with excision wounds. Experimental animals were allocated into several groups, including untreated controls, conventional therapy, and hydrogel treatments with or without the plant extract. Our findings suggest that topical administration of the polyphenol-enriched hydrogel promoted more rapid wound contraction compared with other treatments. This improvement in healing was accompanied by enhanced collagen deposition, reduced oxidative stress, and lower concentrations of pro-inflammatory cytokines. These results indicate that hydrogels combining natural polymers with plant-derived bioactive compounds represent a promising and sustainable approach to regenerative wound care while simultaneously supporting circular economy strategies through the reuse of agricultural residues.

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Invited Talks

Coupled Multicomponent Mixed Oxides based on Alumina: Al_2O_3 -Nd_2O_3 -ZnO-x and Al_2O_3 -Ga_2O_3 -Ag_2O-x, Prepared by the Sol-gel Method, for the Photocatalytic Degradation of Polluting Organic Compounds in Aqueous Media

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Abstract

In spite that alumina is considered as an insulator material, γ-Al_2O_3 prepared by the sol-gel method exhibits high photocatalytic activity in the degradation of organic compounds in aqueous medium. In consequence, γ-Al_2O_3 can be thought as a good option since it is a material of low cost and it has excellent properties such as high specific surface area and good chemical stability. However, one drawback is its high recombination rate of (e^-, h^+) pairs, therefore it is necessary the decrease in the recombination rate to improve its photocatalytic activity. A possible way to decrease the recombination rate of (e^-, h^+) pairs is by contacting γ-Al_2O_3 with lanthanide oxide and by doping it with semiconductor oxides. In this work, coupled multicomponent mixed oxides based on γ-Al_2O_3: Al_2O_3-Nd_2O_3-ZnO-*x* and Al_2O_3-Ga_2O_3-Ag_2O-*x* (Al-Nd-Zn-*x* and Al-Ga-Ag-*x*) were prepared by the sol-gel method and tested in the photodegradation of phenol (80 ppm) and diclofenac (50 ppm) in aqueous media respectively. Al-Nd-Zn-*x* with ZnO concentration in the range 0.8–2.0 wt. % showed high efficacy to degradate phenol, photoconverting about 90 % at 3 h of UV light irradiation. Whereas, Al-Ga-Ag-*x* with Ag_2O concentration between 1.0 and 5.0 wt. % of Ag_2O photoconverts more than 90 % of diclofenac at 20 min of UV light irradiation. The improvement in the photocatalytic activity of coupled Al-Nd-Zn-*x* and Al-Ga-Ag-*x* mixed oxides prepared by the sol-gel method is due to the intimate contact between phases and the high dispersion of ZnO and (Ag^0, Ag^+) species. In both materials, Nd_2O_3, ZnO and Ag^0 and Ag^+ species act as electron traps, whereas Al_2O_3 and Ga_2O_3 act as hole traps, promoting the separation of photoinduced charges and the decrease in the recombination rate of (e^-, h^+) pairs.

Ultrahigh-Strength, yet Tough Nanomaterials by High-Pressure Torsion Deformation of Modest Alloyed Metals

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Abstract

The production of metallic materials contributes largely to the industrial greenhouse gas emission. While increasing their strength would lower the overall materials consumption by smaller component sizes for instance in the mobility, aerospace or energy sector, the necessity for huge alloying contents counteracts a sustainable materials strategy. For ultrahigh-strength levels in steels up to 40% of alloying elements are necessary, making their recycling nearly impossible. Increasing the strength of materials by grain refinement is, thus, the only way to combine two sustainability requirements: i) lower materials consumption for structural components by ultrahigh-strength levels and ii) lean-alloyed materials conditions fostering recyclability and a circular materials industry. Severe plastic deformation is the most efficient and versatile method to synthesize ultrafine-grained and nanocrystalline grain sizes in pure metals. Ultra-high strength levels are thereby achieved by alloying with sub-0.1 wt% of interstitial elements. The major draw-back of this material class lies to date in a lower toughness as compared to conventional structural materials. However, we will present two pathways towards ultrahigh-strength, yet tough and recyclable nanosteels by interface engineering at the nanoscale. Specifically, we will show how modest alloying elements with cohesion strengthening elements like boron can transfer the crack path from the weak boundaries to the grain interior. Furthermore, the introduction of low-energy boundaries [1, 2] maintains high levels of ductility, far beyond of what classical high-angle architectures are able to. A comprehensive experimental approach of severe plastic deformation, high resolution microscopy, atom probe tomography in conjunction to in-situ micromechanical testing will show the great potential of this material class for future materials requirement.

Green Formulation Strategies for Hydrogel Systems: Impact on Antioxidant Activity

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Induction Furnace–Based Valorisation of Steelmaking Byproducts: Case Studies on Mill Scale, Grinding Dust, and ESR Dust

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Abstract:

Steelmaking and secondary processing operations generate large volumes of oxide- and metal-rich byproducts which are often underutilised despite containing significant recoverable value. In this work, the induction furnace (IF) is demonstrated as a viable valorisation technique for such wastes through three case studies: mill scale, grinding dust from valve steel processing, and ESR grinding dust from stainless steel ingots.

For the mill scale case (AISI 4330 V grade), mill scale was converted into carbothermic-reduction briquettes using calcined petroleum coke (CPC) as reductant and molasses as binder. Composition analysis, XRD and TGA were employed to determine suitable carbon addition, with both stoichiometry and TGA indicating that 10–12% carbon yields optimal reduction potential. Subsequent induction furnace trials, involving different charge make-up routes to create a melt pool, showed that using mild steel plates instead of pig iron significantly enhanced recovery. The process achieved recoveries of 99.36% Fe, 75.52% Ni, and 97.01% Mo, with improvements of 24.44% Fe, 14.45% Ni, and 47.47% Mo compared to the pig-iron route. Slag phase analysis via XRD confirmed element losses into oxide phases, and an energy evaluation revealed that the reduction stage accounted for 78.55% of total energy consumption. [1,2]

In the grinding dust case from chromium-rich valve steel, XRF and XRD confirmed high Fe and Cr content. The dust was briquetted using a bentonite binder and processed in an induction furnace, producing ingots containing 94.84% Fe and 4.82% Cr, with mass-balance recovery of 91.44% Fe and 88.91% Cr. For the ESR dust case (SS321 ESR ingot grinding), wet analysis confirmed metallic iron phases in the dust. An induction furnace trial with a 65 kg charge (30 kg electrodes + 35 kg ESR dust) produced alloy-rich ingots, yielding recoveries of 88% Fe, 85% Cr, 93.13% Ni, and 73.1% Mo based on elemental mass balance.[2]

Overall, the results establish induction furnace melting as a scalable route for resource recovery and circular utilisation of steel-industry wastes, enabling high metal recoveries while reducing landfill burden and supporting sustainable steel production.[3]

Keywords: *Recycling, mill scale, induction furnace, briquette, waste utilisation, circular economy*

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Oral Talks

RECYCLING PELLETIZATED WASTE TO PRODUCE INNOVATIVE AND SUSTANABLE CONCRETE

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Abstract

The use of artificial aggregates manufactured from waste and by-product materials, as an alternative to natural aggregates, has attracted considerable research interest.

Extensive research has been conducted to pre-process or pre-treat different source of wastes to be used as raw materials for artificial aggregates (AAs) production. In this experimental work artificial aggregates have been manufactured by means of cold-bonding granulation. Cold-bonding pelletization is carried out through a rotating plate device allowing the formation of pelletized aggregates from waste materials through gravitational and centrifugal forces.

In addition to traditional single step cold bonding granulation, a double pelletization was carried out to reach AAs with improved properties. In the one-step pelletization the waste is incorporated within the binding matrix, while in the two-step pelletization, a second incapsulation is made in order to obtain AAs embedded within an outer shell likely able to improve both their technological and leaching properties.

In this experimental work three types of industrial waste were employed for the production of artificial aggregates: municipal solid waste incineration fly ash (MSWI-FA), ground-granulated blast-furnace slag (GGBFS), and marble sludge (MS).

Several concrete mixtures were designed by alternatively adding either single-bond AAs or double-bond AAs at different dosages (0% - 10% - 20% and 30% replacement by weight of aggregate). All mixtures were prepared with a constant water-to-cement ratio of 0.40, and an aggregate-to-cement ratio of 4.5.

Then, several Artificial Aggregate Concretes (AACs) specimens were manufactured in order to characterize fresh concrete rheological behaviour as well as hardened concrete mechanical and physical properties. In detail, besides to fresh consistency tests, density evaluations were carried out at fresh and hardened state; compression, indirect tensile and bending tests were performed at both early age and long term (3, 7, 28, 90 and 180 days of curing); both secant

static and dynamic elastic modulus by ultrasonic pulse velocity measurements at 28 days of curing were evaluated. Moreover, free drying shrinkage tests up to 180 days under 50% R.H. and 20°C temperature were carried out.

The production of AAs through pelletization proved to be a promising approach. Besides to the improved concrete sustainability, mechanical properties obtained proved to be adequate for use in structural applications.

In particular, the use of double-bond artificial aggregates appears promising, as they improve the interfacial quality between cement paste and aggregate particles, slightly enhance 28-days flexural and tensile strength, and mitigate the negative impact on long-term compressive strength development.

Fabrication of $CeVO_4$@$CePO_4$ Z-Scheme Heterojunction for Highly Efficient Pollutant Degradation: Experimental and DFT Studies

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Abstract

The growing problem of water pollution by harmful contaminants such as pesticides, pharmaceuticals, and dyes, resulting from the activities of many sectors, has become a serious environmental and health issue [1]. Consequently, there is a strong demand for sustainable treatment strategies, most notably advanced oxidation processes (AOPs) and especially photocatalysis, which has become an important approach that uses solar energy for eliminating organic pollutants from water, particularly using advanced semiconductor composite materials with high catalytic activity [2,3].

A well-designed Z-scheme heterojunction improve the separation and transfer of photogenerated electron-hole pairs. CeVO4 and CePO4 prepared by co-precipitation method, were used as precursors to synthesize CeVO4@CePO4 composite *via* a solid-state reaction. In order to correlate the photocatalytic efficiency of the photocatalysts with their structural, morphological, surface chemical, vibrational, and optical properties, the samples were characterized and analyzed using various techniques. Under visible light irradiation, the optimal photocatalyst from the (1-x) CeVO4@xCePO4 series showed a significant improvement in the degradation rate of organic pollutants with excellent recyclability and stability under the tested conditions. The enhanced performance is attributed to improved charge separation and effective light absorption. The optimization process for photodegradation was conducted using response surface methodology (RSM) based on a central composite design (CCD). This statistical approach made it possible to identify significant interactions between operating variable parameters and yielded optimal conditions that maximized degradation efficiency. In parallel, a theoretical study based on density functional theory (DFT) was performed to elucidate the electronic properties of the material and the interaction mechanism involved. These findings provide an integrated experimental and theoretical understanding of the behavior and degradation mechanism using CeVO4@CePO4, contributing to the development of advanced wastewater treatment strategies.

Stabilisation of Dredged Sediment Using Fly Ash and Recycled FRP from Wind Turbine Blades: Strength Development with Magnesium Ammonium Phosphate Cement (MAPC)

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Abstract

This study investigates the stabilization of dredged sediment (DS) using fly ash (FA) and recycled fiber-reinforced polymer (rFRP) from decommissioned wind turbine blades, comparing the mechanical performance of binders based on magnesium ammonium phosphate cement (MAPC) and ordinary Portland cement (OPC). The research responds to two converging challenges: managing large volumes of fine dredged sediment and diverting composite waste from wind turbine blade decommissioning into value-added construction materials. This research presents a comprehensive analysis of particle packing, compaction behavior, early- and medium-age unconfined compressive strength (UCS), stress–strain response, and setting/rheological behavior of MAPC–FA hybrid systems with and without rFRP. Key findings: (1) FA substitution up to 30% by mass improves packing and long-term strength gain in DS matrices; (2) inclusion of 1% rFRP increases peak compressive strength and post-peak toughness; (3) 5% MAPC provides useful early-age strength and ductility compared to 10% OPC, while FA acts to retard MAPC setting and extend workable time; (4) an empirical stiffness–strength relationship was established for the composite materials. The results demonstrate the technical feasibility of producing low-carbon, resilient DS-stabilized materials suitable for non-structural and semi-structural offshore applications and guide further optimization and durability testing.

Keywords: *Dredged sediment stabilization, fly ash, recycled FRP, MAPC, OPC, geopolymer*

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Structural Investigation and Hydrogenation Properties of TiFeCr Alloys

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Abstract

The rapidly increasing global demand for secure and sustainable energy resources has intensified the pursuit of advanced hydrogen storage materials, which are essential for a clean and green energy future. Hydrogen is widely regarded as a next-generation, environmentally friendly energy carrier; however, the development of practical solid-state hydrogen storage systems remains challenging. TiFe-based intermetallics offer advantages such as low cost, moderate operating conditions, and favorable reversible hydrogen capacity. Meanwhile, it remains activation challenge at room temperature.

In this study, adjustment of Ti content and doping Cr are used to solve the activation problem of TiFe-based alloys. We investigate the structural and hydrogenation properties of TiFeCr alloys to address these limitations. Experimental measurements guided the selection of two representative compositions, $Ti_{0.52}Fe_{0.44}Cr_{0.04}\_H_{0.1\text{-}0.5}$, and the Ti-rich δ-phase $Ti_{0.80}Fe_{0.15}Cr_{0.05}\_H_{0.1\text{-}0.5}$, which exhibited superior activation behavior and were therefore chosen for theoretical evaluation.

The ATAT toolkit was employed to generate Monte Carlo Special Quasi-random Structure (MCSQS) supercells by adjusting cluster-correlation weights for each alloy composition. All MCSQS structures were fully relaxed using density functional theory (DFT) to identify the most energetically favorable configurations. Hydrogen atoms were then incorporated into the interstitial sites of these stable structures, with H/M (hydrogen per metal) ratios ranging from 0.1 to 0.5, to determine the enthalpy of hydride formation and the corresponding plateau pressures. Hydrogen loading in pure TiFe over the same concentration range was also examined to provide a reference baseline.

The computational results offer key insights into the thermodynamics of hydrogen absorption and provide theoretical support for the experimentally observed hydrogenation behavior. Overall, the theoretical results closely reproduce the experimentally observed trends, confirming the reliability of the computational approach and highlighting the potential of TiFeCr alloys as efficient and sustainable materials for future hydrogen energy storage applications.

MXene-Based 2D Heterostructures for High-Efficiency Oxygen Evolution Reaction: A First-Principles Study

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Abstract

MXenes, a rapidly growing class of two-dimensional (2D) materials derived from MAX phases and represented by the general formula $M_{n+1}X_nT_x$ (where M is an early transition metal, X is carbon and/or nitrogen, and Tx denotes surface functional groups such as O, F, or OH that tune material properties), have garnered significant attention for photocatalytic applications due to their tunable electronic structure and abundant surface-active sites. Constructing 2D van der Waals (vdW) heterostructures offers an effective approach to promote spatial separation of photogenerated electrons and holes, a key requirement for enhanced photocatalytic efficiency. Designing MXene-based type-II heterostructures remains challenging, as only certain material combinations provide the suitable type-II band alignment. In this work, we performed a first-principles investigation to develop several MXene-based heterostructures by integrating MXenes with Blue Phosphorene (blueP) and transition-metal dichalcogenides (TMDCs). Their photocatalytic potential was systematically evaluated through electronic band gaps (>1.2 eV), band alignment (empirical models and DFT), optical absorption spectra, and Gibbs free energy of reaction intermediates. Phonon dispersion, elastic constants, and ab initio molecular dynamics confirmed the structural and dynamical stability of all systems. Among the investigated vdW heterostructures, MXene/TMDC exhibited outstanding activity toward the oxygen evolution reaction (OER), achieving a low theoretical overpotential of 0.17 eV. For MXene/blueP, biaxial strain further enhanced performance by reducing reaction energy barriers, yielding an OER overpotential of 0.37 eV relative to the unstrained system. These findings highlight MXene-based vdW heterostructures as promising photocatalysts for the OER and demonstrate that interface engineering and strain modulation are effective strategies for designing next-generation energy conversion materials.

Keywords: First principle calculation, Mxene, Blue phosphorous, heterostructure, TMDCs, Photocatalysis, External tuning parameter

Reference: Sarga, P. K.; Karthik, H. J.; Bhattacharyya, S. Electronic and Interfacial Properties of 2D MXene/Blue Phosphorene Heterostructures: Impact of External Strain for Thermoelectric Applications. *ACS Appl. Electron. Mater.* **2024**, *6* (11), 8039–8058. https://doi.org/10.1021/acsaelm.4c01386.

Sustainable 3D Printing of Personalized Dosage Forms Using Biomass-Derived PLA Filaments

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Abstract

The pharmaceutical sector faces mounting pressure to reduce its environmental footprint while responding to the growing demand for personalized therapies and resilient healthcare delivery systems. Conventional, centralized drug manufacturing relies on energy-intensive processes, standardized dosage forms, and long distribution pathways, leading to excessive material waste, high carbon emissions, and limited adaptability to individual patient needs. These challenges are further intensified by demographic changes, rising healthcare costs, and the need for rapid, localized responses to fluctuating demand. As a result, there is an urgent need for alternative production paradigms that integrate sustainability, digitalization, and patient-centric design within pharmaceutical manufacturing and distribution.

The 3D-SustainDrugs project proposes a transformative model for pharmaceutical production based on decentralized, on-demand manufacturing enabled by three-dimensional (3D) printing technologies and embedded within neighbourhood pharmacy networks. Focusing on solid oral dosage forms of Non-Steroidal Anti-Inflammatory Drugs (NSAIDs), with indomethacin as a model compound, the project develops sustainable, customizable drug delivery systems produced *via* fused deposition modeling (FDM). Central to this approach is the use of bio-based and waste-derived materials, including polylactic acid (PLA) synthesized from amylaceous biomass and activated carbon derived from pyrolyzed olive pits, combined into biodegradable composite filaments suitable for pharmaceutical 3D printing

Beyond technological development, 3D-SustainDrugs integrates comprehensive sustainability assessment throughout the product life cycle by systematically capturing environmental, economic, and social indicators such as energy consumption, CO_2 emissions, material efficiency, and waste generation. By linking material properties, printing parameters, and drug performance with sustainability metrics, the project establishes a data-driven framework for optimized, low-impact pharmaceutical manufacturing. The proposed model enables precise dose personalization, reduced overproduction, minimized logistics requirements, and late-stage customization at or near the point of care.

By combining digital manufacturing, biomass valorization, and localized production, 3D-SustainDrugs advances a novel vision for neighbourhood pharmacies of the future, positioning them as active micro-manufacturing hubs within resilient healthcare ecosystems. The project contributes to the broader objectives of Industry 5.0 by aligning technological innovation with environmental responsibility, social value creation, and regional economic development, offering a scalable pathway toward sustainable, patient-centered pharmaceutical systems in Europe and beyond.

Cervicare: Advancing Point-of-Care Diagnostics for Cervical Cancer

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Abstract

Cervical cancer, predominantly caused by High-Risk Human Papillomavirus (HR-HPV) type 16, remains a formidable global health challenge due to its high mortality rates. Despite medical advancements, traditional cervical cancer detection methods suffer from inefficiencies and cost limitations. To address this critical need, our study focuses on the development of an innovative electroanalytical genosensor.

Our novel genosensor is based on $Ti_3C_2T_x$/DNA hybrid screen-printed paper electrode strips, specifically designed for the detection of HPV-16, a primary risk factor for cervical cancer. Leveraging the unique properties of MXene nanostructures, we enhance sensor performance. Comprehensive characterization techniques, including X-Ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), Fourier Transform Infrared Spectroscopy (FTIR), and UV-Visible Spectroscopy (UV-Vis), provide insights into crystal structure, surface morphology, functional groups, and optical properties.

The genosensor demonstrates highly sensitive detection capabilities. Evaluated using Cyclic Voltammetry (CV) analysis, it exhibits an impressively low Limit-of-Detection (LoD) of 2.4 fM for HPV-16 DNA. Integration with cutting-edge technology results in the creation of the Cervicare device, a portable, user-friendly solution with an LoD of 0.02 pM. This device holds promise for point-of-care diagnostics, especially in remote areas.

Cervicare represents a significant leap forward in cervical cancer screening. By providing a rapid, accurate, and affordable diagnostic solution, it holds the potential for earlier detection and improved disease management. Its practicality and suitability for resource-constrained settings make it a powerful tool in enhancing healthcare accessibility.

Analcime Zeolite from Natural Silica and Coal Fly Ash: Taguchi-Based Optimization and Adsorption Study

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Abstract

Zeolites are valuable nanomaterials widely used in selective adsorption, ion exchange, and heterogeneous catalysis. Due to the growing demand and high cost of conventional precursors, low-cost and abundant raw materials are increasingly required. This study investigates the zeolitization of natural silica and coal fly ash using an L9 Taguchi orthogonal array to optimize synthesis parameters: NaOH concentration, synthesis time, hydrothermal temperature, and SiO_2/Al_2O_3 mass ratio. The obtained powders were characterized by XRD, FTIR, SEM/EDX, and DTA/TG. Zeolitization efficiency was evaluated through ANOM/ANOVA analyses. Optimal conditions (160 °C, 36 h, 1.5 M NaOH, SiO_2/Al_2O_3 = 2.2) yielded 89% efficiency, with analcime as the main phase. The adsorption performance of the optimal sample toward methylene blue showed pseudo-second-order kinetics and good agreement with Langmuir, Freundlich, and Temkin isotherms. A removal efficiency of 99.69% was achieved under optimal conditions.

Valorization of Phosphate Sludge through Silica Recovery: A Sustainable Approach to Transform Overlooked Mining Waste into Wealth

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Abstract

Silica nanoparticles (NPs) are widely valued for their multifunctionality, yet their conventional production relies on resource-intensive processes with considerable environmental burdens. In light of these considerations, this study proposes an innovative valorization pathway in which phosphate sludge (PS), an abundant and environmentally problematic by-product of phosphate beneficiation, is transformed into high-purity nano-silica through sol-gel extraction process applied to this largely overlooked resource. The PS samples were initially treated with hydrochloric acid at concentrations of 1 %, 3 % and 5 % to eliminate metal and phosphate impurities. Then the resultant silica-rich solid served as the feedstock for synthesizing silica NPs, which were comprehensively characterized using multiple analytical techniques. The results demonstrate that high-purity amorphous silica microspheres (98.25-98.69 % SiO2) were successfully produced. XRD pattern exhibited a broad peak centered at $2\theta \approx 22.5°$, indicating its amorphous structure. The particles exhibited a narrow size distribution with an average diameter of 40–50 nm and a high SSA ranging from 2323.54 to 354.7 m2/g. Furthermore, FTIR spectra exhibited well-defined vibrations associated with Si-OH and Si-O-Si, demonstrating the progressive condensation of the silica network. Thermal analyses revealed a robust mesoporous framework that remained stable up to 600 °C, together with the presence of both physically absorbed and structurally bound water. SEM further evidence that the product consisted of compact clusters of well-dispersed nanoparticles, thereby confirming the nanoscale and homogeneous nature of the obtained silica. The measured point of zero charge (pHpzc) of 9.1 highlights the surface chemistry of the synthesized silica and its potential suitability for applications requiring controlled surface reactivity. Owing to its unique characteristics, the produced silica offers substantial potential for a wide range of applications, including advanced ceramics, adsorption and catalysis, polymer reinforcement, and energy storage systems. This work therefore provides a promising pathway for the large-scale valorization of phosphate sludge, contributing simultaneously to resource recovery and environmental sustainability.

Poster Presentations

Chemical Extraction of Valuable Components from End-of-life Photovoltaic Cells

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Abstract

Recycling of photovoltaic modules at the end of their service life is becoming increasingly important amid the rapid growth of installed solar energy capacity. Crystalline silicon solar cells contain valuable metals, primarily silver and copper, whose recycling helps reduce environmental impact and dependence on primary resources. This paper presents an experimental approach to extracting silver and copper from spent solar cells using an ammonia-peroxide system in a batch reactor. Hydrogen peroxide acted as an oxidant, converting the metals into ionic forms, while ammonia promoted the formation of stable, soluble ammine complexes of silver and copper. The solution was applied in excess of the metal content in the processed material, allowing evaluation of the process's efficiency without the chemical limitations imposed by the reagents.

Experimental data showed that metal dissolution is limited in the initial stages of the process. The maximum silver recovery during the first hours of the reaction was approximately 5% of its calculated content in the sample. For copper, this figure did not exceed 1% over the comparable period. The results indicate that the process is limited by kinetic and diffusion factors, as well as metal surface passivation, rather than by a lack of reagents.

Despite the low recovery rate in the early stages, the ammonia-peroxide system demonstrates selectivity for silver and potential for further process intensification. Optimising temperature, processing time, material pretreatment, and mass transfer conditions can significantly increase copper and silver recovery and ensure the industrial applicability of the proposed photovoltaic waste recycling technology.

Employing Bio-inspired Lone Pair-π Interactions in Sequestration and Activation of Environmentally Detrimental Molecules

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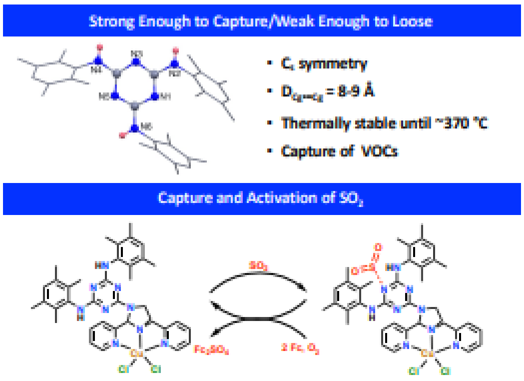
Abstract

Noncovalent interactions (NCIs) are ubiquitous and crucial in stabilizing biomolecules, host-guest chemistry, and supramolecular assemblies. These interactions include hydrogen bonding, π-π stacking, cation-π, anion-π, and lone pair-π interactions. While most of these interactions are well-studied, lone pair-π interactions have yet to be observed in action, especially in sequestration chemistry. In this work, we investigate the utility of lone pair-π interactions as a sustainable and efficient mechanism for stabilizing and capturing toxic, volatile, and smallmolecule pollutants. Herein, we synthesized a symmetrical trisubstituted 1,3,5-triazine molecular system as a stable host that can form piedforts with sufficient inter-disc spacing (~9 Å) between two C_3N_3 rings to park environmentally detrimental molecules such as DCM, SO_2, CS_2, and VOCs. Tri-substituted triazines with hydrophobic peripheries enable the tuning of the inter-disc distance between adjacent C_3N_3 rings and the interaction between neighboring molecules. The resulting interaction between the host and the gaseous guest molecule was minimal, that were just strong enough to capture a guest molecule but sufficiently weak to permit its release with minimal energy input. Accordingly, the host-guest interaction remained marginal, enabling efficient capture and facile release under mild thermal or pressure changes. Single-crystal X-ray diffraction (SCXRD) analysis confirms the presence of intermolecular lone pair-π interactions between the triazine ring centroid and electronegative atoms of detrimental molecules, validating the proposed recognition mechanism. The thermal stability of host-guest complexes was studied by thermogravimetric analysis, and it was found that guest molecule retention even above the boiling points of the molecules.

Furthermore, the triazine-appended copper (II) koneramine complex $[Cu(L^{Tz}\text{-}H)Cl_2]$ was designed to bind SO_2 and facilitate its oxidative conversion to sulfate through efficient electron transfer from ferrocene. The SO_2 binding coupled electron transfer (SOCET) process from the ferrocene was confirmed through control experiments alongside techniques such as electronic absorption spectroscopy, cyclic voltammetry, and electrospray ionization mass spectrometry. Overall, these results establish lone pair-π interactions as a powerful bio-inspired strategy for capturing, stabilizing, and transforming harmful small molecules, offering new opportunities for green chemistry and sustainable environmental remediation.



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Charging Rate Dependence of Lithium Ion Transfer at Positive Electrode/Solid Electrolyte Interfaces in all Solid State Lithium Ion Rechargeable Batteries

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Abstract

The All-solid-state lithium (Li)-based batteries (ASSB) have been expected as next generation rechargeable batteries with high energy density, long-life performances in addition to safety aspects. The positive and negative electrodes/solid electrolyte (SE) interfaces in the ASSB have the highest resistance and dominate for the characterization of the Li^+ ion conduction, resulting in the reduction of the battery capacity. In particular, understanding dynamic behaviors of Li^+ ions at the interfaces is so essential to realize the development of the ASSB by a fast charging.

The aim of this work was to investigate in-situ the changes in the Li concentration around the $LiCoO_2$ positive electrode/LATP($Li_{1+x+y}Al_xTi_{2-x}Si_yP_{3-y}O_{12}$) SE interfaces under slow and fast charging conditions using elastic recoil detection (ERD) to clarify the charging rate dependence of the Li^+ ion transfer between $LiCoO_2$ positive and in-situ formed LATP negative electrodes in the ASSB.

The ASSB samples of Au/$LiCoO_2$/LATP/Pt multilayers with Au and Pt current collectors were fabricated using the magnetron sputtering and applied by 2.8 V at slow and fast charging rates of 0.31 and 1.56 mV/s. The ERD spectra revealed that the Li concentration, x, in Li_xCoO_2 decreased with increasing the applied voltages and eventually became approximately 0.10 and 0.59, respectively, for 2.8 V at the slow and fast charging rates. The much amounts of Li^+ ions accumulated at the $LiCoO_2$/LATP interface by the fast charging rate cannot insert due to lattice expansion as an intercalation, resulting in diffusing in the opposite direction of each positive and negative electrode to reduce the battery capacity.

Encapsulation of Residual Microalgal Biomass to Produce Slow-release Fertilizer for Hydroponic Systems

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Keywords: hydrogel, slow-release biofertilizer, nutrients reclamation, circular bioeconomy

Abstract

During the last decade, the global fertilizer price has been continuously increasing, leading to great concerns on food security. Microalgae-derived biomass waste generated from microalgal-industries during the production of biostimulants is considered as a promising source of alternative fertilizers because it contains valuable nutrients such as nitrogen and phosphorus and several bioactive compounds. Herein, we presented a **novel strategy for the production of slow-release biofertilizers by encapsulating residual microalgal biomass in alginate-based hydrogels.** The well-prepared hydrogel-coated pellets with a thin and thick coating layer (2 and 4 mm after swelling) were applied as slow-release fertilizers to cultivate basil and lettuce in hydroponic systems with tap water and commercial liquid fertilizers as controls. The plant growth profiles and water quality parameters in hydroponic systems were monitored periodically. The preliminary results showed that (1) the hydrogel could well encapsulate microalgal pellets with **excellent stability (remaining its structure for ~30 days in distilled water).** Hydrogels showed high swelling capacity, with thicker coatings retaining more water than thin coating. (2) Within the initial 2 h, thick and thin hydrogel-coated biomass pellets showed **slower nutrient release rate for TN and phosphate** than the raw biomass residuals in DI water. Reducing coating thickness led to a higher nutrient release rate. (3) When the thin hydrogel-coated biomass pellets were used as fertilizers for the hydroponic system, the basil plants showed higher growth and yield than those plants grown with the commercial fertilizer solution after 64-days of cultivation. Whereas, lettuce plants grown with both thin and thick hydrogel-coated biomass pellets displayed relatively less plant height, leave number and leaf length compared to those with the fertilizer after 67- days of cultivation. The findings of this project support **nutrient reclamation** from microalgal industrial waste and the advancement of a **circular bioeconomy.**

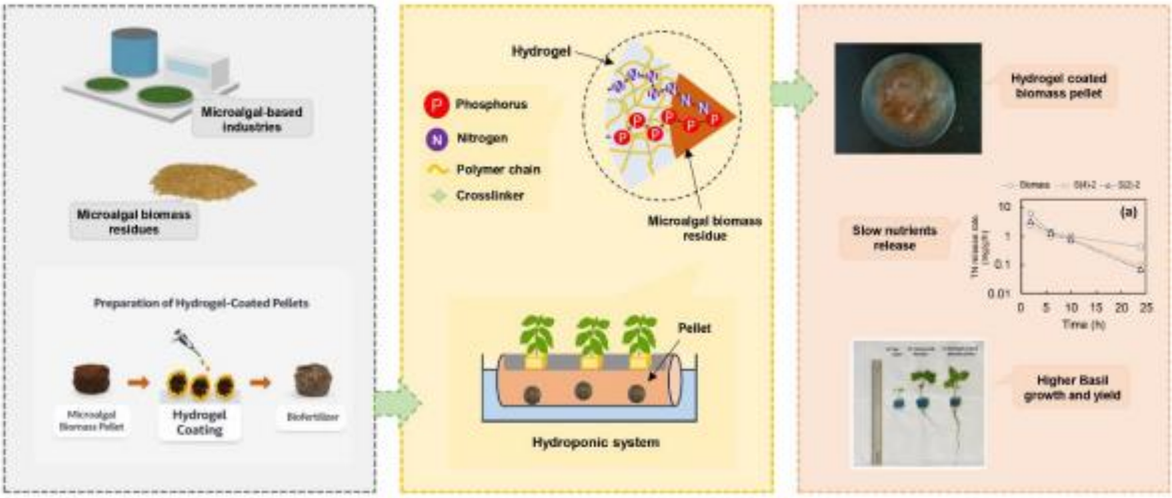

Figure. *Production and utilization of hydrogel-coated biomass pellet in hydroponic system for vegetable cultivation.*

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