22nd International Symposium on Intercalation Compounds

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Clermont-Ferrand, France
July 6-10, 2025

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Program

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Sunday, July 6th, 2025

TIME	EVENT
18:00 - 22:00	Registration and Welcome Party, Clermont-Ferrand City Hall

Monday, July 7th, 2025

TIME	EVENT
08:00 - 08:30	Registration Desk
08:30 - 08:45	Opening Ceremony
08:45 - 09:35	Invited Lecture - Rachid YAZAMI - Chairwoman : Katia Araujo da Silva
09:35 - 10:25	Plenary Lecture - Sébastien CAHEN - Chairwoman : Katia Araujo da Silva
10:25 - 10:45	Coffee break
10:45 - 12:45	Oral Communications - Chairman : Sébastien Cahen
10:45 - 11:05	› Phase diagram of Li-graphite intercalation compound formed by the charge/discharge reaction in Li-ion batttery - *Hiroyuki Fujimoto, Kyoto University Gokasho, Uji Campus*
11:05 - 11:25	› Optimization of hard carbon porosity via pressure-assisted pyrolysis for enhanced sodium storage - *Oumaima Hatim, Institut Jean Lamour*
11:25 - 11:45	› Graphite fluoride as lithium primary battery active material for spacecraft applications - *Régis Porhiel, Institut de Chimie de Clermont-Ferrand*
11:45 - 12:05	› Charge transfer in alkaline-earth metal graphite intercalation compounds: combination of experience and calculation - *Lucie Speyer, Institut Jean Lamour*
12:05 - 12:25	› Biomolecule intercalated layered materials: Understanding bonding, structure and reactivity in cationic and anionic host-guest complexes - *H. Christopher Greenwell, Department of Earth Sciences, Durham University*
12:25 - 12:45	› Exploration of Na-Mn-O system: toward new cathode materials for sodium-ion batteries? - *Tanguy SOUDANT, Laboratoire de cristallographie et sciences des matériaux, Réseau sur le stockage électrochimique de l'énergie*
12:45 - 14:15	Lunch
14:15 - 14:50	Keynote Lecture - Kostas DEMADIS - Chairwoman : Chiara Bisio
14:50 - 15:50	Oral Communications - Chairwoman : Chiara Bisio
14:50 - 15:10	› One-pot mechanochemical synthesis of phosphate-intercalated hydrocalumite - *Heloise Pastore, Institute of Chemistry, University of Campinas*
15:10 - 15:30	› Surface Modification of Carbon Nitrides for Enhanced Photocatalytic Hydrogen Production - *Jae-Hun Yang, Global Innovative Center for Advanced Nanomaterials (GICAN), College of Engineering, Science and Environment, The University of Newcastle, Callaghan, NSW 2308, Australia*
15:30 - 15:50	› Novel synthetic route of titanium phosphates and phosphonates for drug intercalation - *Elena De Paolis, University of Perugia, Department of Pharmaceutical Sciences*
15:50 - 16:20	Coffee break
16:20 - 17:00	Oral Communications - Chairman : Kostas Demadis
16:20 - 16:40	› Elaboration of layered double hydroxide films with photoactive antibacterial properties - *Sushant Sharma, Laboratoire de Chimie Physique et Microbiologie pour les Matériaux et l'Environnement (LCPME), UMR 7564*
16:40 - 17:00	› Layered double hydroxides intercalated with fluoride as a filler of polymer composites for dental use - *Piccinini Michela, Department of Pharmaceutical Sciences, University of Perugia*
17:00 - 17:20	› Insight on the photocatalytic properties of Zn-based LDH derived mixed oxide toward degradation of persistent herbicide in water - *Hao Wang - Institut de Chimie de Clermont-Ferrand*
17:20 - 17:40	› Physico-chemical phenomena during acidic leaching of positive electrode materials in the context of Li-ion batteries recycling - *Anne Héloïse FOLGADO, PHysicochimie des Electrolytes et Nanosystèmes InterfaciauX, Réseau sur le stockage électrochimique de l'énergie*
17:40 - 17:50	ISIC web site presentation - ISIC web site presentation
17:50 - 18:15	Exhibitors Presentations - Exhibitors Presentations
18:15 - 21:00	Poster Session – Wine and Cheese Party

Poster Session

POSTER N°	TITLE, AUTHOR, LABORATORY (COUNTRY)
P01	> CFD Simulation of Multifluid Mixing in A Rotating Liquid Film Reactor for Magnesium Hydroxide Production,Lin Yanjun, State Key Laboratory of Chemical Resource Engineering (China)
P02	> Zirconium phosphates and sulfophosphonates intercalated by guanidine synthesis, characterization and ionic conductivity,Tomáš Plecháček, University of Pardubice (czech republic)
P03	> Assembly of intercalated Layered Double Hydroxides with "fence" structure for enhancing anti-migration performance,Li Dianqing, State Key Laboratory of Chemical Resource Engineering (China)
P04	> The effect of the electrolyte concentration on the performances of Layered Double Hydroxides intercalated with Ferrocene anions,Douard Camille, IMN CNRS (France)
P05	> Ecologically Friendly 2D/2D Na+-MXene/LDH for Cesium Adsorption in Salt Lakes: A Comprehensive Study on Adsorption Performance, Mechanisms, and Environmental Impact,Gao Li, School of Mechanical Engineering, Qinghai University, Xining (China)
P06	> Enhanced CO2 Hydrogenation Performance of Fe/Co-Based Nano Hydrotalcites for carbon neutral Fuels synthesis: A Study on Ultrasound-Assisted Synthesis and Catalytic Efficiency,Di Michele Alessandro , Department of Physics and Geology, University of Perugia (Italy)
P07	> Enhanced Anti-Migration of Organic Antioxidants via Chitosan-Encapsulated Ultrathin Intercalated Layered Double Hydroxides Fabricated by a Nucleation-Encapsulation Coupling Strategy,Li Zijia, Beijing University of Chemical Technology (China)
P08	> Topochemical silanization of the Aurivillius phase Bi2SrTa2O9 and post-synthesis complexation of the interlamellar spacing,Chapel Pacôme , Institut de Physique et Chimie des Matériaux de Strasbourg (23 rue du Loess - BP 43 - 67034 Strasbourg Cedex 2 - France France)
P09	Preparation of inorganic nanosheets and their application as high barrier packaging films, Fan Siyuan , China University of Geosciences (China)
P10	> Sonochemical and mechanochemical as green routes for the preparation of layered double hydroxides,Nocchetti Morena, Department of Pharmaceutical Sciences, University of Perugia, Via del Liceo, Perugia (Italy)
P11	> Construction of inorganic confining structures in layered double hydroxide interlayers for enhancing anti-migration performance,Wang Liren, State Key Laboratory of Chemical Resource Engineering (China)
P12	> Synthesis and Characterization of Calcium Hydroxyapatite Composites Enhanced with Isoeugenol for Antibacterial Activity,Karciauskaite Justina , Institute of Chemistry, Vilnius University (Lituany)
P13	> Coordination Stabilization of Fe by Porphyrin-intercalated NiFe-LDH under Industrial-level Alkaline Conditions for Long-term Electrocatalytic Water Oxidation,Hu Yihang , Beijing University of Chemical Technology (China)
P14	> Intercalation of photosensitizers in Zn2Al-layered double hydroxide for water remediation,Roche Laura , Laboratoire de Chimie Physique et Microbiologie pour les Matériaux et l'Environnement (France)
P15	> single component, single layer flexile foam evaporator with the higher efficiency for water generation,Li Ruoxin, State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing(China)
P16	> Highly Luminescent Organic Phosphors Confined in LDH: A Rare-Earth Free Alternative for Solid-State Emission,Zerbib Guillaume , Institut de Chimie de Clermont-Ferrand (France)
P17	> Bimetallic synergistic effect of Co and Fe for the highly efficient catalytic decomposition of ozone,Liu Wendi, State Key Laboratory of Chemical Resource Engineering (China)
P18	> Tailoring LDH Morphologies for Advanced Catalytic and Antibacterial Applications,Boccalon Elisa, Department of Chemistry, Biology and Biotechnology, University of Perugia (Italy)
P19	> Study of the high-pressure structure of fluoroperovskite : the lamellar post-perovskite,Pelat Lucas , Institut de Chimie de Clermont-Ferrand (France)

POSTER N°	TITLE, AUTHOR, LABORATORY (COUNTRY)
P20	> Preparation of Well-defined Anatase Nanoparticles in a Nanoporous Polyimide Membrane for the Uniform Deposition of Platinum,Vejchakul Krittachai, Ogawa Makoto, Vidyasirimedhi Institute of Science and Technology (Thailand)
P21	> Preparation and characterization of new layered zirconium aminophosphonates,Melanova Klara, University of Pardubice (czech republic)
P22	> Design of new luminescent hybrid materials based on layered oxides,Lépée Ludovic, Institut de Physique et Chimie des Matériaux de Strasbourg (France)
P23	> First preparation of fluorinated diamane-type materials by ball-milling in a liquid phase, Haddad Guillaume, Institut de Chimie de Clermont-Ferrand (France)
P24	> Application of layered and porous materials of biogenic origin in the removal of heavy metals and organic pollutants from water,Marchesi Stefano, University del Piemonte Orientale (Italy)
P26	> Use of the Memory Effect of Hydrotalcites for the Preparation of Composite Anion Exchange Membranes for Electrolysis, Donnadio Anna , Department of Pharmaceutical Sciences, University of Perugia (Italy)
P27	> Highly Exposed Low-Valence Ni sites of NiO(111) for Efficient Electrocatalytic Biomass Upgrading,Z. Song, State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, (China)
P28	> Simultaneous Mineralization of Cd(II), Pb(II) and As(V) Using MgAl-NO3: Performance and Mechanism, Haoran Wang, State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, (China)
P29	> Ultrathin NiV Layered Double Hydroxide for Methanol Electrooxidation: Understanding the Proton Detachment Kinetics and Methanol Dehydrogenation Oxidation,Z. H. Wu, State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, (China)
P30	> Synthetic Application of Immobilized Chiral Secondary Amine Catalysts and Impregnated Palladium Nanoparticles, Kamlar Martin, Charles University, Faculty of Science, Prague (czech republic)
P31	> The formation of monetite on the synthesis and dehydration of brushite, Héloïse Pastore, Institute of Chemistry, Universidade Estadual de Campinas, Campinas (Brazil)

Tuesday, July 8th, 2025

TIME	**EVENT**
08:00 - 08:30	Registration Desk - registration desk
08:30 - 09:20	Plenary Lecture - Luyi SUN - Chairman : Seong-Ju Hwang
09:20 - 10:00	Oral Communications - chairman : Seong-Ju Hwang
09:20 - 09:40	› LDHs as cargo for luminescent compounds: a case study with original click fluorophores - *Federico Cisnetti, Institut de Chimie de Clermont-Ferrand*
09:40 - 10:00	› Layered double hydroxide based luminescent materials - *Dongpeng Yan, Beijing Normal University*
10:00 - 10:30	Coffee break
10:30 - 11:05	Keynote Lecture - Nathalie STEUNOU - Chairman : Luyi Sun
11:05 - 12:25	Oral Communications - Chairman : Luyi Sun
11:05 - 11:25	› Conjugated phthalocyanine based mesoporous covalent organic framework for efficient negative electrode lithium storage - *Rong Jiang, Rong Jiang*
11:25 - 11:45	› Delaminated alk-MXene/Co-MOF composite membranes for high-efficiency removal of Cr(VI) and Tetracycline - *Wei Wang, Beijing Key Laboratory of Environmentally Harmful Chemical Analysis, Beijing University of Chemical Technology, Beijing 100029, China*
11:45 - 12:05	› Dirac metals for two-dimensional MoS2 semiconductors as excellent electrode - *Katsumi Tanigaki, BAQIS*
12:05 - 12:25	› Intimately mixed copper, cobalt, and iron fluorides resulting from the insertion of fluorine into a LDH template - *Abderraouf Rouag, Institut de Chimie de Clermont-Ferrand*
12:25 - 12:45	Symposium Picture - official picture
12:45 - 14:15	Lunch
14:15 - 14:50	Keynote Lecture - Joao TEDIM - Chairwoman : Nathalie Steunou
14:50 - 15:50	Oral Communications - Chairwoman : Nathalie Steunou
14:50 - 15:10	› Superconductivity of alkali C60 fullerides viewed from electrical conductivity - *Xinying Li, Beijing Academy of Quantum Information Sciences (BAQIS), Beijing National Laboratory for Condensed Matter Physics; University of Chinese Academy of Science, Beijing 100190, China*
15:10 - 15:30	› New ways to intercalate corrosion hydroxyquinoline-based inhibitor molecules in LDH: paradigm changes in synthesis protocols - *Julien SARMET, Institut de Chimie de Clermont-Ferrand*
15:30 - 15:50	› Preparation of Layered Double Hydroxides with Varied Layer Charge - *Makoto Ogawa, Vidyasirimedhi Institute of Science and Tecchnology, Shinshu University*
15:50 - 16:20	Coffee break
16:20 - 18:00	Oral Communications - Chairman : Makoto Ogawa
16:20 - 16:40	› Anomalously large thermoelectric Seebeck observed in intrinsic organic semiconductors - *Shilin Li, Beijing Academy of Quantum Information Sciences, Beijing, China, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Science, Beijing; University of Chinese Academy of Science, Beijing*
16:40 - 17:00	› Visualizing Atomic Quantum Defects in Ultrathin 1T-PtTe2 - *Junhai Ren, Beijing Academy of Quantum Information Sciences, 100193 Beijing, China*
17:00 - 17:20	› Micron-Scale antioxidant Intercalated layered double hydroxides for enhanced gas barrier and thermal stability in polyurethane composites - *MH Zhao, State Key Laboratory of Chemical Resource Engineering, College of Chemistry, Beijing University of Chemical Technology*
17:20 - 17:40	› Innovative soft chemistry approach for cation insertion in layered perovskite oxides: chemical and multi-technique structural investigation - *Pacôme CHAPEL, Institut de Physique et Chimie des Matériaux de Strasbourg*
17:40 - 18:00	› Dual-Metal-Substituted Ruthenate Perovskite Oxide for Efficient Alkaline Hydrogen Evolution - *Yiyang Sun, Yonsei University*

wednesday, July 9th, 2025

TIME	EVENT
08:30 - 09:20	Plenary Lecture - Veronica de ZEA BERMUDEZ - chairman : Joao TEDIM
09:20 - 10:20	Oral Communications - Chairman : Joao TEDIM
09:20 - 09:40	› Screening the potential of Prussian blue analogues for novel proton batteries - *Valentin DAMOUR, Institut de Chimie de la Matière Condensée de Bordeaux*
09:40 - 10:00	› Solar hydrogen production under the Caribbean sun - *Jorge Colón, University of Puerto Rico-Rio Piedras*
10:00 - 10:20	› Layered Double Hydroxides as Hosts for Controlled Nutrient Release in Sustainable Agriculture - *Cristina Neves, CICECO – Aveiro Institute of Materials*
10:20 - 10:50	Coffee break
10:50 - 12:30	Oral Communications - Chairwoman : Veronica de ZEA BERMUDEZ
10:50 - 11:10	› Defect and Interface Engineering in Two-Dimensional Inorganic Nanosheet-Based Electrocatalysts - *XIAOYAN JIN, University of Seoul*
11:10 - 11:30	› Different porous adsorbents for PFAS removal from aqueous solutions - *Federico Begni, Nano-SiSTeMI Center*
11:30 - 11:50	› PoLA (Porosity Local Analysis): An Accurate Descriptor of Microporous Volume to Predict Gas Adsorption in Porous Carbons - *Cossi Maurizio, Università del Piemonte Orientale - Dipartimento DISIT Italy*
11:50 - 12:10	› Single-component and binary H2O and CO2 co-adsorption isotherm model on amine-functionalised Mg-Al mixed metal oxides - *Zhuozhen Gan, Shanghai Jiao Tong University*
12:10 - 12:30	› In situ capture of initial nucleation particles for layered double hydroxides - *Yanan Liu, State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing 100029, Quzhou Institute for Innovation in Resource Chemical Engineering, Quzhou, Zhejiang Province, 324000*
12:30 - 14:00	Lunch
14:00 - 18:00	Visits and excursions - Visit in or around Clermont-Ferrand
20:00 - 23:00	Gala Diner

Thursday, July 10th, 2025

TIME	EVENT
08:30 - 09:20	Plenary Lecture - Pilar ARANDA - Chairwoman : Heloise PASTORE
09:20 - 10:30	Oral Communications - Chairwoman : Eloise PASTORE
09:20 - 09:40	› Organic-inorganic hybrids having a talc-like structure as hosts for light-driven applications - *Jocelyne Brendlé, Institut de Science des Matériaux de Mulhouse, UMR UHA CNRS 7361*
09:40 - 10:00	› Preparation of novel synthetic saponite clays from agricultural rice husk and their application for the abatement of organophosphorus pesticides - *Stefano Marchesi, Università del Piemonte Orientale - Dipartimento di Scienze e Innovazione Tecnologica*
10:10 - 10:30	› Preparation and characterization of a monolithic composite composed of geopolymers and layered double hydroxides (LDH) for simultaneous immobilization of ions in an alkaline environment - *Yunge Bai, Institut de Chimie de Clermont-Ferrand*
10:30 - 10:50	Coffee break
10:50 - 11:50	Oral Communications - chairwoman : Pilar ARANDA
10:50 - 11:10	› Optimized Synthesis of Organic-Inorganic Hybrids having Talc-like Structure for Organic Molecules Intercalation - *Ali Dhaini, Institut de Science des Matériaux de Mulhouse*
11:10 - 11:30	› 2D Inorganic Nanosheets and Nanohybrids for Energy Storage Technologies - *Seong-Ju Hwang, Yonsei University*
11:30 - 11:50	› Advances in antioxidant Intercalated Layered Double Hydroxides for Polyolefins - *Yongjun Feng, State Key Laboratory of Chemical Resource Engineering, College of Chemistry, Beijing University of Chemical Technology*
11:50 - 12:20	closing Ceremony

A new method for fast charging Lithium ion batteries

Rachid YAZAMI*

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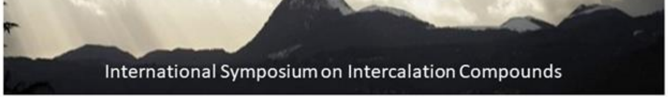
Lithium ion batteries (LIB) use lithium intercalation materials for the cathode and anode. Currently, two cathode materials have become the most popular, which are the lithiated nickel, manganese, cobalt oxide (NMC) with 2D crystal structure and the lithium iron phosphate (LFP) of 3D olivine structure. The anode is mostly based on graphite although a small fraction of other elements such as silicon are used.

The common charge method of LIB is based on applying a constant current (CC) until a voltage is reached then, either that end voltage is applied (CCCV) or the CC is reduced until a new end voltage is reached (MSCC). Both CCCV and MSCC methods apply well as long as the full charge time (0-100% state of charge SOC) keeps below about 1 hour. Should charge time be reduced, the general tendency is the LIB will heat up, which poses a serious safety risk.

Here we introduce a new method for fast charging LIB based on non-linear voltammetry (NLV). In NLV current is never constant by following the chronoamperometry kinetics rules at any applied constant voltage (CV). A series of CV steps are applied while the flowing charge current is controlled until a new voltage step is applied. Within each CV step the current goes to zero for a very short time called rest.

WE will show that NLV not only enables ultra fast charging of some specific LIB cells and packs (down to 6 min full charge), but also NLV enables the extension of the LIB lifespan due to moderate heating during charge and enhances the LIB energy density and safety.

All these advances in the LIB management will be illustrated during the presentation together with some ideas on using artificial intelligence methods to further improve the NLV method



Intercalation into carbon materials: way of synthesis, structural and physical properties, and application for alkali-ion batteries

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Intercalation chemistry can be realized in numerous varieties of organic and inorganic materials, from three-dimensional to 0D materials. Especially, carbon presents a wide variety of allotrops (graphite, carbon nanotubes, fullerene and other nanocarbons, disordered carbons…) which can be used as intercalation host for numerous invited species. Intercalated carbons and carbon-based materials are involved in many fields: design and synthesis strategies, environment, health, engineering, composites, catalysis, energy … Among this so impressive number of possibilities, graphite remains a particularly interesting case.

During this lecture, the different ways of synthesis of so-called Graphite Intercalation Compounds (GIC) will be presented, that cover one century of evolution. It will be shown that solid-gas, solid-liquid and solid-solid reactions can be realized in order to prepare high quality bulk intercalated compounds.

Then, we will illustrate how GIC can be considered as model materials for the demonstration of staging phenomenon, topotactic reactions and electronic charge transfer that systematically happens upon this type of intercalation chemistry. Selected examples will be detailed for the illustration of the structure-physical properties relationships. On a fundamental point of view, intercalation into other carbon materials will also be presented in comparison with graphite.

Finally, we will show how far intercalated carbon materials that can be graphitized or not are so precious materials for sustainable technologies such as alkali-ion batteries.

Tailoring the morphology of MOF nanocrystals by using self-assembled materials

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Precise control over nanomaterial morphology and dimensions is crucial for tuning their physico-chemical properties. Advances in DNA and protein nanotechnology, inorganic crystallization, and polymer/surfactant self-assembly have enabled unprecedented synthesis of anisotropic nanoparticles—such as 1D nanotubes, nanowires, 2D platelets, rings, and stars.[1] This crystal engineering has not only enabled the exploration of novel physical, chemical, and biological phenomena but also spurred the development of advanced applications. In recent decades, MOFs have attracted considerable interest, as this family of porous solids offers a unique opportunity to design a wide range of architectures with modulated porosities and chemical functionalities. Most MOF research has focused on discovering new structures, assessing their properties, and developing MOF-based composites, while less attention has been paid to the control of MOF crystal size and morphology. Progress in this area has primarily relied on carefully chosen synthesis conditions and the use of structure-directing agents or modulators. [2,3] However, these methods often yield powdered samples consisting of spherical, isotropic nanocrystals with limited size control. The rare existing 1D MOF architectures in the forms of nanowires, nanotubes and nanorods were synthesized through a bottom-up solution route or hydrothermal process eventually templated by polymer or inorganic 1D nanostructures. [3,4]

Herein, we present our progress in the development of MOFs based composites to address environmental and energy-related applications. The assembling of MOFs with biopolymers and carbon based materials was envisaged not only to process MOFs composites and impart novel functionalities but also to control the diameter/shape of MOFs nanocrystals and their spatial organization within the support matrix.[5,6,8] We have taken profit of the self-organization properties of biopolymers and carbon-based materials and liquid-liquid phase separation processes to tune the organization, nanostructuration and porosity of composites.[5-8] Advanced characterization tools (X-ray diffraction, N_2 porosimetry, TEM analytical and imaging techniques, HAADF-STEM, electron diffraction…) were combined to provide a complete picture of these composites at the nanoscale and describe their mechanical, interfacial and dynamic properties. Recently, by using graphene oxide nanoscrolls as structure directing agents, a series of 1D Al MOFs nanostructures differing in their crystal dimension and aspect ratio as well as structural flexibility upon guest molecules adsorption have been prepared.[5,8] All these materials were investigated for the capture of pollutants, gas separation or (bio)catalysis.[5-7]

References

[1] A. K. Pearce, T. R. Wilks, M. C. Arno, R. K. O'Reilly, *Nat. Rev. Chem.* 2021, 5, 21–45.
[2] L. Feng, K.-Y. Wang, J. Willman, H.-C. Zhou, *ACS Cent. Sci.* 2020, 6, 359–367.
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[4] K. Dassouki, S. Dasgupta, E. Dumas, N. Steunou, *Chem. Sci.* 2023, 14, 12898–12925.
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Phase diagram of Li-graphite intercalation compound formed by the charge/discharge reaction in Li-ion batttery

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Abstract

Precision chronopotentiometry was performed for a negative graphite electrode in Li-ion batteries by varying the current load during the charge/discharge process. The differential capacity *dQ/dV* with respect to the potential *V* was then calculated. As the current load decreased, the *V-dQ/dV* curve profile changed depending on the current, the reduction peak split, and elementary reaction analysis during intercalation became possible. When these results were combined with operando synchrotron X-ray diffraction measurements, a phase diagram of Li-GIC was established, as shown in Fig. 1. Because graphite has an extremely high anisotropy, structural analysis usually only provides information on the stacking direction. Here, by focusing on the in-plane superlattice group formed by the rearrangement of Li ions, information was obtained about the in-plane direction of the graphite that clarified the intercalation behavior.[1,2]

Acknowledgments

This work is based on results obtained from a project, JPNP16001, commissioned by the New Energy and Industrial Technology Development Organization (NEDO). The synchrotron radiation experiments were performed on the BL28XU beamline at the SPring-8 facility with the approval of the Japan Synchrotron Radiation Research Institute (JASRI) .

References

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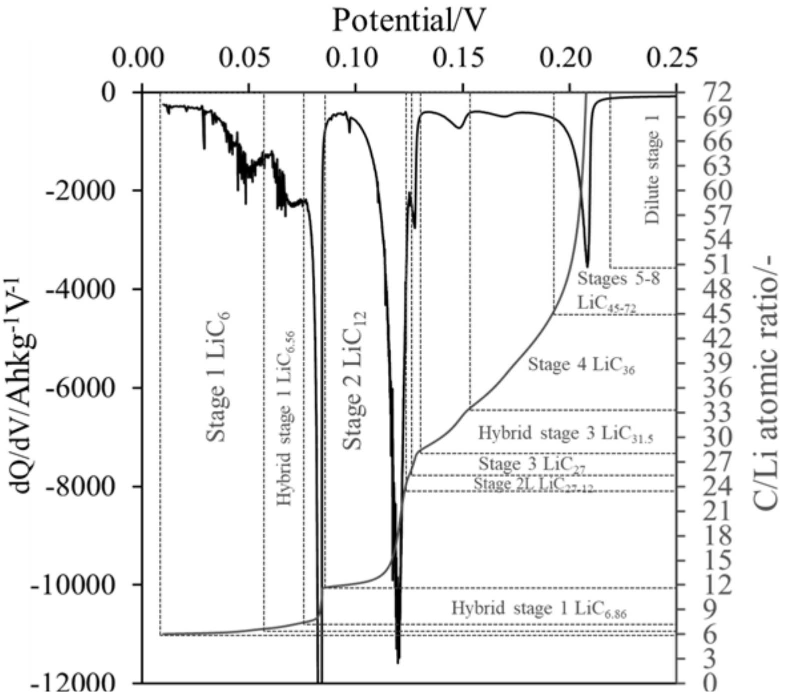
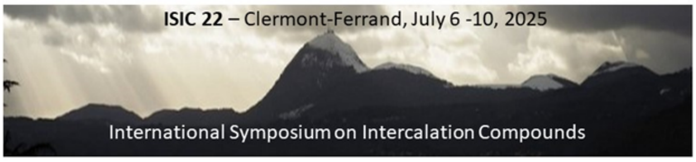


Fig. 1 Phase diagram of Li-intercalated graphite in terms of V-dQ/dV and V-C/Li curves.



Optimization of hard carbon porosity via pressure-assisted pyrolysis for enhanced sodium storage

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With the growing need for efficient and sustainable energy storage, sodium-ion batteries (NIBs) are emerging as a viable alternative to lithium-ion batteries (LIBs) due to the abundance and lower cost of sodium. However, one of the key challenges remains the development of suitable anode materials. Graphite, commonly used in LIBs, is not effective for sodium storage [1]. Hard carbons have gained interest as promising candidates thanks to their disordered structure and porous network, which can accommodate sodium ions through multiple storage mechanisms, including adsorption, intercalation, and pore filling.

Among the factors influencing their electrochemical performance, porosity plays a crucial role**.** Recent studies suggest that closed porosity provides essential low-potential storage sites for sodium, directly impacting capacity and cycling stability [2]. Traditionally, achieving this specific porosity requires high-temperature pyrolysis (~1400°C), which increases energy consumption and limits large-scale production. Raspado *et al*. [3] demonstrated that pressure-assisted pyrolysis effectively controls porosity evolution, enhancing sodium storage properties in sucrose-derived hard carbons.

Building on this approach, our work explores the influence of different biomass-derived precursors, including fructose and lignin**,** to assess how precursor chemistry impacts pore formation and electrochemical performance. By varying synthesis conditions, we aim to further understand the role of closed porosity and optimize hard carbon materials for sodium-ion storage while maintaining a lower processing temperature.

Hard carbon materials were synthesized under different pressure conditions and characterized through structural, textural, and electrochemical analyses. Our results show that while the chemical composition and graphitic ordering remain largely unchanged, the pore network is significantly affected by the synthesis conditions. Electrochemical tests confirm that pore structure optimization influences sodium storage capacity.

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Graphite fluoride as lithium primary battery active material for spacecraft applications

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Lithium batteries are interesting for space applications because they allow energy storage with high density. For applications such as deep space exploration, the battery will be used years away, too far from the sun to be associated with solar panels (*e.g.* for exploration of Europe, Jupiter's satellite, the battery will be used only after approx. 10 years, after travelling the 780.10^6 kilometers from Earth to Europe). Primary batteries are therefore used because they allow higher energy densities compared to secondary batteries.[1]

For these applications, sub-fluorinated graphite (CFx, 0<x 1) are particularly interesting electrode materials with high energy density (up to 2180 Wh kg-1) and good stability over time (<0.5 % self-discharge per year).[2] The graphitic precursor, the synthesis protocol of the CFx powder, the mechanical grinding of the CFx, the formulation protocol of the CFx electrodes as well as the electrolyte composition are important parameters that directly affect the electrochemical performance of CFx//Li cells.[2-4]

This study aims to find the best parameters for the synthesis of CFx obtained by direct fluorination of expandable graphite, as well as the mechanical, formulation and electrolyte parameters to maximise the electrochemical performances. The obtained and scaled-up CFx//Li will then be discharged in "operational" conditions to simulate the experienced conditions of a deep space mission (*i.e.* with low temperature, high radiation environment and power densities required to operate the equipment on board).

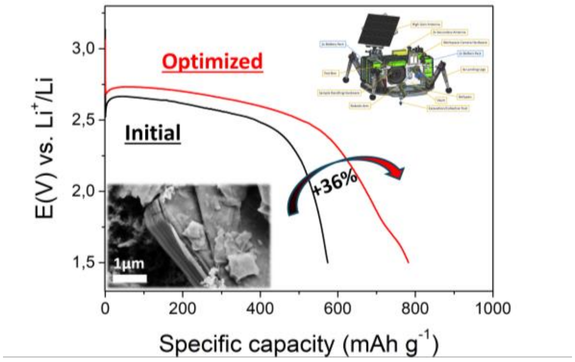

Figure 1. Galvanostatic discharge of CFx//Li (black curve) and optimized CFx//Li (red curve) cells at D/80 discharge rate with SEM picture of the CFx electrode in the bottom left inset and a design model of a lander in the upper left inset[1]

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Charge transfer in alkaline-earth metal graphite intercalation compounds: combination of experience and calculation

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Alkaline-earth graphite intercalation compounds (GIC) raise interest from a fundamental point of view for the study of low-dimensionality materials, but also with more applicative perspectives with the intensive researches about metal-ion batteries. They result from a RedOx reaction, through an electron transfer between metal atoms and graphene layers. This feature is extensively studied because essential to understand the properties of alkaline-earth-based GIC, especially their superconductive behavior. In this work, we propose the combination of both experimental and calculation approaches [1].

The experimental part of this study is carried out with high-quality first-stage bulk CaC_6, SrC_6 and BaC_6 samples, elaborated with different targeted techniques. X-ray diffraction (Figure 1a) allows to quantify charge transfer through the variation of the lattice parameter *a*, which is modified as electrons leave the metal to settle on graphene layers [2]. Raman spectroscopy (Figure 1b) brings complementary information thanks to the modification of spectra and the appearance of new vibration modes [3]. These results highlight a decreasing charge transfer with the electron-phonon coupling as the size of the intercalant and the GIC interplanar distance increase.

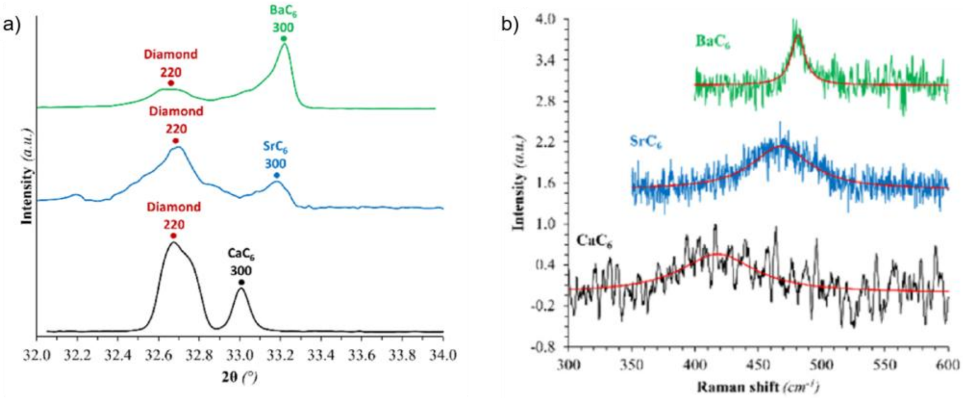

Figure 1. a) X-ray diffractograms of CaC_6, SrC_6 and BaC_6 with diamond powder as internal standard to accurately measure the ***a*** parameter. b) Raman spectra of CaC_6, SrC_6 and BaC_6: focus on the C_z band whose position varies with charge transfer.

Experimental results are combined with a modeling approach. Electronic structures, charge density profiles and band structures are determined with first-principles DFT calculations using the QUANTUM-ESPRESSO code [4]. Calculated results are in good agreement with experimental ones, and confirm the evolution of the charge transfer with the chemical nature of the alkaline-earth intercalant.

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Biomolecule intercalated layered materials: Understanding bonding, structure and reactivity in cationic and anionic host-guest complexes

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Through intercalation and ion exchange processes, layered minerals are implicated in governing a number of biogeochemical cycles in nature, as well as controlling the transport and fate of xenobiotic molecules in the environment. In industry, layered intercalated minerals find numerous technological applications, including as hosts for delivery of biomolecules in therapeutics. The intercalation properties of layered minerals are embedded at an atomic scale, with the identity and location of isomorphic substitutions and structural defects influencing charge density, ion exchange and acid/base reactions, as well as the interlayer spacing.

Owing to their low crystallinity, and layered nature, understanding the structure of layered minerals presents a number of challenges. Experimental techniques give insights into bulk mineral crystal structure and reactivity, and advanced microscopy methods are increasingly able to address external surface structure and phenomena. However, the interfacial region, and especially the interlayer region of layered minerals is difficult to characterise by experimental methods. The dynamics and reactivity of the interlayer region, especially with either low numbers or mixtures of guest molecules, or for those with complex guest molecule structures such as biomolecules remain a challenge.

Computational chemistry methods applied to layered minerals have given exceptional insight into the “hidden” world of intercalated molecule structure, dynamics and reactivity. Here we describe the results of a number of studies of the structure, material properties, intercalation mechanisms, stability and reactivity of nucleic acid and amino acid intercalated layered materials using both computational and experimental methods.

Exploration of Na-Mn-O system: toward new cathode materials for sodium-ion batteries?

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Today, society is increasingly dependent on electricity. In response to climate change, governments around the world are promoting the development of green mobility (electric and hybrid vehicles) as well as the production of electricity from renewable sources (hydraulic, wind, solar, etc.). However, the drawback of this type of production is its dependence on weather conditions. To smooth out production when it exceeds demand, or vice versa, the use of electrochemical storage is necessary. Currently, this market is largely dominated by lithium-ion (Li-ion) technology. The lack of real alternatives is causing strain on raw materials (lithium, cobalt, and even graphite). In response to the challenges related to resources, sodium-ion (Na-ion) batteries, which rely on a much more abundant element than lithium, represent a promising alternative. In addition, manganese oxides are of great interest because of manganese's abundance, low toxicity, and cost-effectiveness. For these reasons, we embark us to develop a new cathode material based on sodium and manganese oxides.

The Na-Mn-O system includes numerous phases, with many compositions reported in the 70's primarily as single crystals for the most part. To date, the two most extensively studied phases used as cathode materials for sodium-ion batteries are Na_xMnO_2 [1-3] and $Na_2Mn_3O_7$ [4,5]. Among all the known compositions, the phase $Na_{10}Mn_4O_9$ attracts our interest for several reasons. By assuming the reversible extraction and insertion of height sodium ions, the theoretical capacity can reach 360 mAh/g. In addition, its unique crystal structure is particularly intriguing. Indeed, edge and corner-shared $[MnO_4]$ tetrahedral are forming a kagomé-type layered structure together with isolated $[MnO_3]$ trigonal planar units. This is the only representative of this type of trigonal coordination in the Na-Mn-O system [6].

Therefore, in this presentation, we will discuss a comprehensive study of the intercalation compound $Na_{10}Mn_4O_9$, which includes solid-state synthesis, as well as magnetic and electrochemical characterizations.

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One-pot mechanochemical synthesis of phosphate-intercalated hydrocalumite

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Hydrocalumites are a class of layered double hydroxides known for their versatility. Their ability to exchange interlayer anions with external ones gives these materials favorable properties for both the removal and controlled release of these species. Although a wide range of organic and inorganic anions can be accommodated in the interlayer space, intercalation strategies depend on the nature of the anion.

The most common methods for intercalation rely on ion exchange in solution, which can occur either directly or indirectly. In direct intercalation, the target anion is incorporated into the structure during synthesis, whereas in indirect intercalation strategies may require ion exchange and structural reconstruction through the memory effect. This work proposes the one-step synthesis of the phosphate-intercalated hydrocalumite.

This synthesis strategy involves mechanically inducing the one-pot formation of phosphate-intercalated hydrocalumite. The reagents were milled using a ball mill with agate spheres during the following periods of time: 30 min, 1 h, and 2 h. The formation of the desired structure and the success of the synthesis were corroborated through X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FTIR).

The quantification of both intercalated and free phosphate was carried out using the standard addition method coupled with XRD. The presence of a characteristic peak around 2 θ = 28.5º associated with KCl, indicated phosphate intercalation within the interlayer space. It is worth mentioning that solid-state synthesis offers significant advantages, including reduced solvent usage, minimized synthetic steps, and the prevention of other undesirable calcium phosphate phases, such as hydroxyapatite and brushite, which commonly occur when ion exchange is performed in solution.

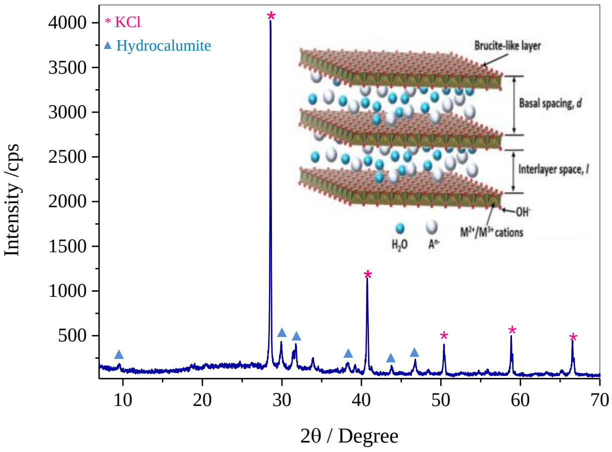

Figure 1: XRD pattern of the synthesized P-hydrocalumite sample. Insert graph represents the general structure of LDHs[4].

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Surface Modification of Carbon Nitrides for Enhanced Photocatalytic Hydrogen Production

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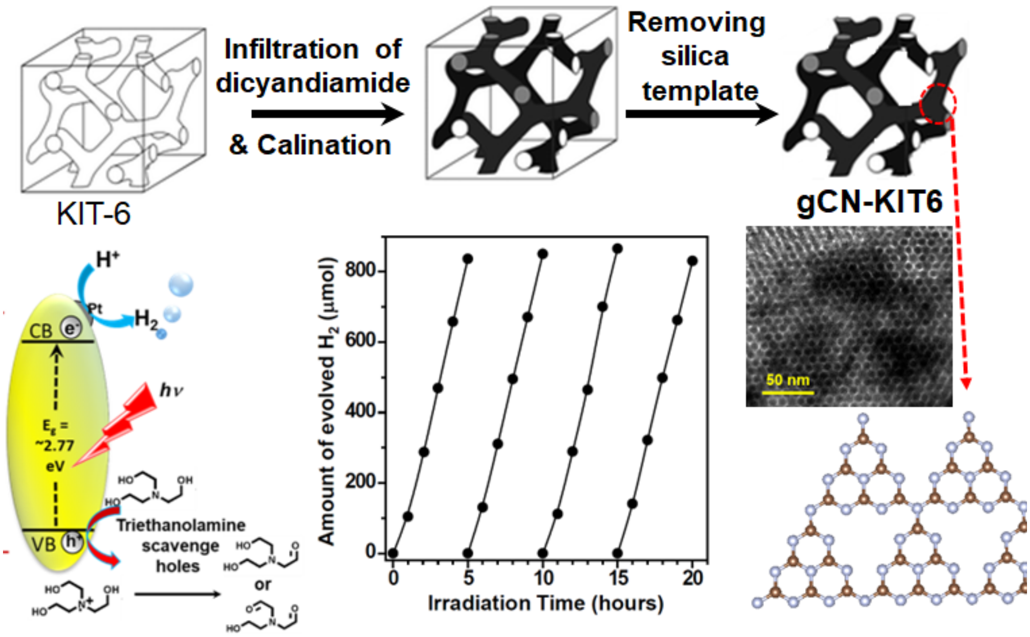
Hydrogen production via photocatalysis has attracted significant attention as one of the most promising and sustainable approaches due to its clean reaction process, which utilizes only water and solar energy with photocatalyst materials. Carbon nitrides, metal-free catalysts with visible light-harvesting semiconductor, can be synthesized from abundant carbon and nitrogen resources, and have been utilized as photocatalysts for sustainable hydrogen production. However, the challenges including rapid electron-hole recombination kinetics, low charge transfer efficiency, and limited surface area significantly restrict the efficiency of photocatalytic water splitting for hydrogen production. In this study, we report several strategies to address these challenges: (1) synthesizing carbon nitrides with porous texture to increase surface area, leading to enhancing the number of active sites on the carbon nitride photocatalyst surface, (2) forming crystalline carbon nitride structures to improve electron-hole transfer efficiency, and (3) designing C-doped carbon nitride, where the π-electron density is precisely tuned. These approaches optimize band positions, reduced electron-hole recombination kinetics and enhanced conductivity, significantly boosting hydrogen production from splitting water under simulated solar light. The physico-chemical properties of the engineered carbon nitrides were characterized using various analytical techniques, such as X-Ray diffraction, transmission electron microscopy, X-ray photoelectron spectroscopy, near-edge X-ray absorption fine structure spectroscopy, and photoluminescence spectroscopy along with theoretical calculations. These surface-engineered carbon nitride photocatalysts will bring us to realizing a green hydrogen economy.



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Novel synthetic route of titanium phosphates and phosphonates for drug intercalation

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Metal phosphonates are lamellar compounds with an astonishing ability to intercalate different kinds of molecules. Their main exponent is the well-known zirconium phosphate, but there are other promising yet overlooked metal phosphates, the first being titanium phosphate. α-Ti $(HPO_4)_2$•H_2O (TiP) is a α- Zr $(HPO_4)_2$•H_2O (ZrP) isomorph and presents higher intercalation capability and cytocompatibility than ZrP [1], making it very interesting for drug delivery. The synthetic routes of this material usually employ highly reactive precursors, such as $TiCl_4$ or titanium alkoxides that make difficult to control the particle size and morphology. In order to improve these aspects and in the context of sustainability and scalability, novel synthetic approaches for TiP are investigated, based on sol-gel procedures and mechanochemistry, by using a $Ti^{IV}O$ based salt, aliphatic alcohols and concentrated phosphoric acid. Preliminary results highlighted interesting results in terms of particle morphology. Structural and physico-chemical characterization, as well as the study of intercalation and functionalization properties of the prepared materials are under investigation.

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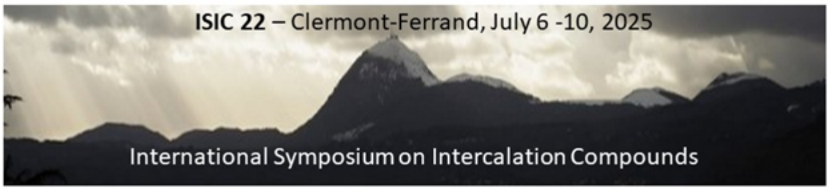

Elaboration of layered double hydroxide films with photoactive antibacterial properties

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Layered double hydroxides (LDH) have gained significant attention as promising photoactive materials [1] for antibacterial applications [2]. These two-dimensional hydrotalcite-like materials, with the general formula $[M^{2+}_{1-x}\ M^{3+}_{x}\ (OH)_2]^{x+}\ \ [(A^{n-})_{x/n.}\ y\ H_2O]^{x-}$, consist of anions A^{n-} sandwiched between positive brucite-like sheets containing divalent M^{2+} and trivalent M^{3+} cations. Interestingly, by altering the composition of the octahedrally centered divalent and trivalent cations, these materials can be photoactive. Two types of photoactivity can be obtained: the generation of reactive oxygen species (ROS) [3] by photocatalytic process in the UV-visible region and/or heat by photothermal behavior [4]. Both properties can be used to cause damages to bacterial cells. Moreover, the intrinsic antibacterial nature of certain substituted divalent cation (e.g. Zn^{2+}, Cu^{2+}) [5], when combined with their photoactive properties, can also lead to an amplified bactericidal effect. Developing these LDH in the form of film is ideal for antibacterial assays. The growth of LDH as films [6] favours precise morphological control and easy retention after use. To harness these advantages, we have optimised the synthesis of different LDH films on aluminium-based substrates. Using hydrothermal routes and different precipitants (ammonia, urea), we have obtained LDH films with different compositions (M^{2+}=Cu/Zn/Co). The as-synthesized films are characterized primarily by X-ray diffraction and vibrational spectroscopies (Infrared and Raman) to confirm the LDH phase and determine the intercalated anions. The film morphology was analyzed by Scanning Electron Microscopy. Diffuse Reflectance Spectroscopy was used to determine the optical properties. The elementary composition was determined by X-ray Photoelectron Spectroscopy and Energy Dispersive X-ray Spectroscopy. These films were evaluated for their photoactivity upon light irradiation both for ROS production and photothermal effect. *E. coli* bacteria were exposed to the LDH films surface, and antibacterial property was evaluated in absence and presence of light by classical microbiological methods involving Colony Forming Units counting, diffusion into agar and epifluorescence microscopy.

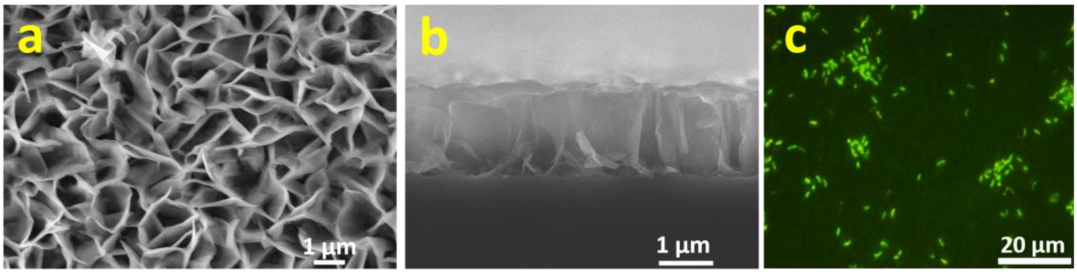

Figure 1**:** (a) Top-view and (b) cross-section Scanning Electron Microscopy images of ZnAl LDH film. (c) Epifluorescence image depicting *E. coli* on LDH surface after LIVE/DEAD™ *Bac*Light™ staining.

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Layered double hydroxides intercalated with fluoride as a filler of polymer composites for dental use

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In recent years, there has been an increased need to use new materials in dentistry that have adequate mechanical strength, biocompatibility, antibacterial and remineralization properties.
In this context, the utilization of layered double hydroxides (LDHs) as fillers in polymers such as poly(dimethacrylate)s (PMMA) and Ethylene Vinyl Acetate (EVA) has obtained particular interest.
LDHs are a class of 2D materials consisting of positively-charged host layers and exchangeable interlayer anions, which can be expressed by the formula $[M(II)_{1-x}M(III)_x(OH)_2](A^{n-})_{x/n}$ x mH_2O where M(II) and M(III) are divalent and trivalent metals, respectively and A^{n-} is the interlayer anion.
The potential for intercalating LDHs with fluorides (LDH-F) has proven to be a particularly advantageous method for fabricating materials that can be utilized as filler polymers. This approach enables the controlled and gradual release of fluorides, thereby facilitating their application in various dental products, including removable dentures and composite in restorative dentistry. The presence of fluorides has been demonstrated to exert a substantial influence on numerous facets of dental care, including the promotion of remineralization of the mineral phase of damaged teeth and the facilitation of antibacterial action through the inhibition of microorganism metabolism [1].
LDH-F functionalized on the surface with methacrylate anions (LDH-F/MA) was utilized as filler of PMMA for the fabrication of dental filling materials [2]. Composites loaded with LDH-F/MA at 5 wt% showed good mechanical properties, high fluoride release and the ability to recharge fluoride when contacted with fluoride solution. A filler consisting of LDH-F and silica (LDH-F/SiO_2) was developed with the aim of producing resin composites with a high filler content, low polymer shrinkage and improved mechanical properties. This filler allowed to reach 40% of inorganic load in the PMMA maintaining adequate amount of fluoride in the composite.
Another application of LDH-F was its integration within polymers to fabricate dental splints and aligners, with the objective of mitigating bacterial infections that frequently manifest as a consequence of these appliances. To obtain this aim, ZnAlGa LDH in nitrate form was prepared and the nitrate anions were exchanged with fluorides. Finally, the LDH was incorporated into EVA, and the resulting material was characterized and evaluated for its mechanical and antibacterial properties against *C. albicans*.

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Insight on the photocatalytic properties of Zn-based LDH derived mixed oxide toward degradation of persistent herbicide in water

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Layered Double Hydroxides (LDHs) containing transition metals are materials with tunable chemical compositions and unique lamellar structure. They have received extensive advertence in recent years due to their photoactivity, and particularly in the photocatalytic degradation of various pollutants through advanced oxidation processes (AOPs). Upon thermal treatment, the layered structure of LDHs collapses, leading to the formation of non-stoichiometric, metastable mixed metal oxides with semiconducting properties. Such chemical transformation can enhance photocatalytic performance by increasing the surface area and improving redox properties [1].

In this study, a series of Zn_2Al_1-Cl-LDOs photocatalysts was synthesized via a coprecipitation method and subsequently calcined at different temperatures (300, 500, and 700°C). These materials were then employed as persulfate (PS) photoactivators to degrade chloridazone (CLZ), a selective herbicide belonging to the pyridazinone-derived pesticide class [2].

Photocatalytic performance of those Zn_2Al_1-Cl-LDOs was evaluated through the degradation of CLZ with/without PS under UVA irradiation. As shown in Fig.1, Zn_2Al_1-Cl-500°C/PS/light system exhibited the highest degradation efficiency achieving 94.3% CLZ removal within 4h. XPS, photoluminescence and radical quenching experiments confirmed that oxygen vacancy (V_o) generated during calcination facilitated the separation and transfer of charge carriers, while also playing a key role in activation of PS to generate $HO^\bullet$ and $SO_4^{\bullet-}$ radicals, the main active species involved in CLZ degradation. Moreover, the effects of operational parameters such as catalyst and PS dosage, initial pH, intercalated anions and trivalent metal cations were investigated. In summary, this work provides insights into the relationship between the structural features of Zn-based LDOs and their photocatalytic performance, with potential implications for the design of efficient photoactivators for environmental remediation.

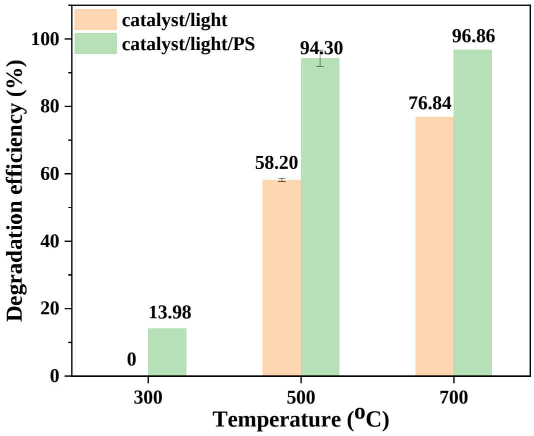

Fig.1. Effect of different calcination temperatures on CLZ photodegradation with/without PS

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Physico-chemical phenomena during acidic leaching of positive electrode materials in the context of Li-ion batteries recycling

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Positive electrode materials used in LIB mostly rely on lithiated transition metal oxide whose constituents are increasingly critical due to the deployment of large-scale batteries. Because of their limited cycle life, batteries recycling has been an increasing field of research often seeking to optimize processes. In hydrometallurgy, leaching step enables to dissociate elemental constituents to enable their re-use [1]. Due to the low solubility of lithiated metal oxide in aqueous medium, this step is often conducted in highly concentrated acid [2]. It involves many physico-chemical phenomena that are difficult to capture as they occur at spatial and temporal multi-scale.

To better understand the overall picture of dissolution mechanism in lithiated transition metal oxide, we sought to probe the reactivity of both the liquid and solid scale. Using the prototype compound $LiMn_2O_4$, we developed an adapted protocol based on in situ conductivity measurement relying on the significant differences in molar ionic conductivity [3] of proton (350 $cm^2.\Omega^{-1}.mol^{-1}$) and the released species: Li^+ (38.6 $cm^2.\Omega^{-1}.mol^{-1}$) and Mn^{2+} (107 $cm^2.\Omega^{-1}.mol^{-1}$). The experimental data have been interpreted using a kinetic model allowing to assess rate constants and activation energy. By combining this study with ex situ characterization (XRD, TEM, elemental analysis), we will discuss in this presentation, a revised model of Hunter [4] providing novel insight into dissolution mechanism.

Key words: Recycling, leaching, dissolution, conductivity, Li-ion battery, intercalation compounds.

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LDHs as cargo for luminescent compounds: a case study with original click fluorophores

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This study explores the intercalation of novel sulfonated organic fluorophores, based on a mesoionic triazolium backbone (**triaz**), into layered double hydroxides (LDHs). The fluorophores are easily synthesized on a gram-scale using *Click* Chemistry approaches[1].

Sulfonation of the scaffold was efficiently performed using sulfuric acid with two examples of different steric bulk. The resulting sulfonated fluorophores, highly soluble in aqueous basic solutions (deprotonated NH, anionic form), were co-immobilized into ZnAl LDH host structure by coprecipitation with either dodecyl sulfate (DS) or phenylene dipropionate (PPA). The efficiency of the fluorophore loading was assayed by fluorescence spectroscopy. PPA, thanks to its size, rigidity and bi-functionalized (pillar-effect) nature, enabled more efficient fluorophore insertion than DS. It was demonstrated that optimal interlamellar spacing (size-matching of the PPA spacer and the luminescent host – so called SMIS design) is essential.

The study reveals that the integration of the **triaz1** molecules considerably improves their luminescence properties, notably by reducing the aggregation-caused quenching (ACQ) typical of organic fluorophores in their solid form. Samples intercalated with PPA exhibit optimal luminescence in the blue region, with external quantum yields up to 55% under UV excitation [2].

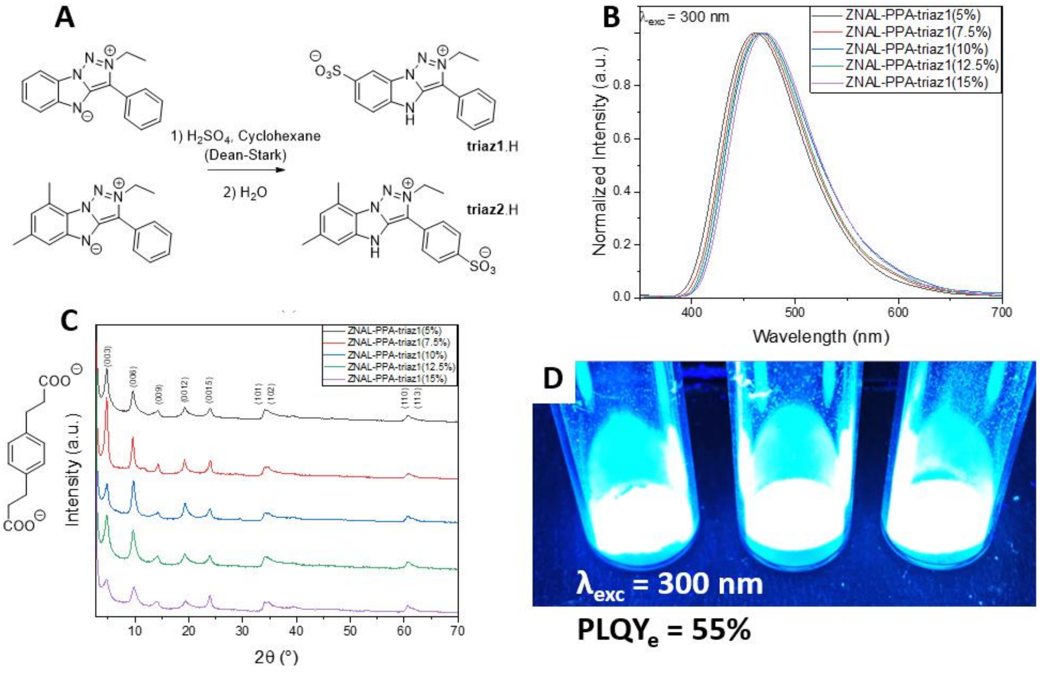

Figure 1. A: sulfonation reactions. B, C fluorescence spectra and PXRD data of LDH loaded with triaz. D. Photographs of **triaz**-loaded ZnAl-LDH powders under UV excitation

The approach yielded similar intercalation results with the **triaz2** fluorophore, demonstrating the robustness of our design and its flexibility in adjusting emission wavelengths. This is in line with previous results from our laboratory on different families of luminescent compounds [3] and paves the way for applications in 3D printing, which will be preliminary discussed during this presentation.

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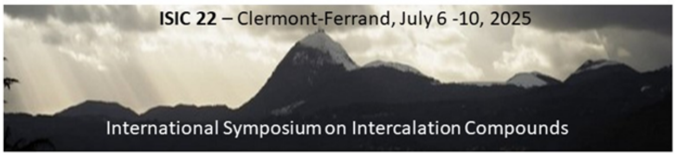

Layered Double Hydroxides Based Luminescent Materials

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Construction of the layered structures has been an effective way to achieve new luminescent materials for sensors, optical display, biological imaging and therapy applications. In this work, we reported the fast development of layered double hydroxides (LDHs) based luminescent materials, particularly for the tuning of their excited states are reviewed. Firstly, the relationship between the structures and luminescent performances of the LDHs host-guest materials and their sensor properties are introduced. Attention then mainly focuses on the tuning of singlet and/or triplet excited states of the LDHs-based luminescent materials. Finally, we briefly discuss the new host-guest fluorescent and long-lived phosphorescent materials with stimuli-responsive performances.

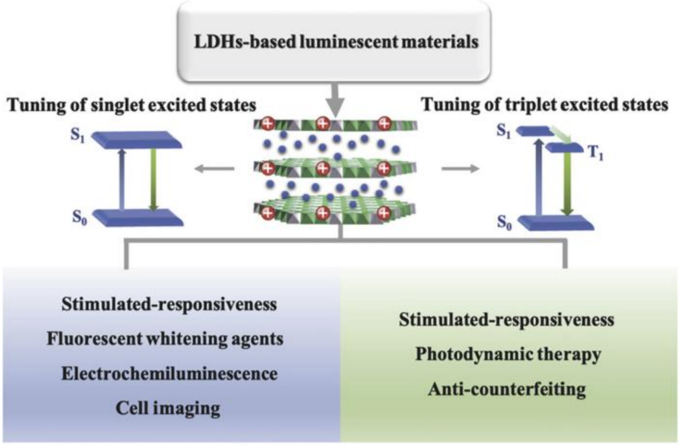

Figure 1. Tuning of the excited states of LDHs intercalation materials

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Conjugated phthalocyanine based mesoporous covalent organic framework for efficient negative electrode lithium storage

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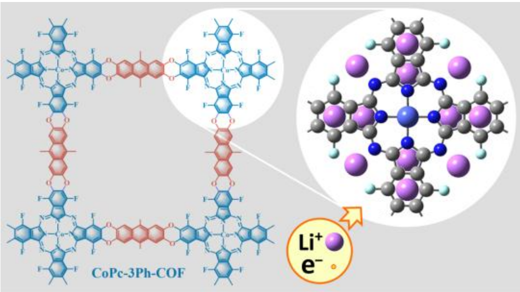
Traditional organic negative electrode materials have received widespread attention due to their significantly higher theoretical capacity than graphite, particularly in terms of structural diversity, designability, and resource sustainability.However, the low conductivity and small pore size of organic compounds limit their practical applications, often leading to disadvantages such as poor cycling stability. COFs are a new type of porous crystalline polymer with many advantages such as high specific surface area, long-range ordered structure, and adjustable pore size. Compared with traditional organic small molecules, COFs have lower solubility in electrolytes due to their stable framework structure. In particular, the high specific surface area of COFs can promote interface contact between electrodes and electrolytes, and the adjustable pore size of COFs can accelerate ion insertion/extraction processes, thereby improving Li^+storage performance. In addition, the π-π stacked layered structure of two-dimensional (2D) COFs endows them with better conductivity, which is beneficial for the rapid storage of Li^+. In this study, two conjugated phthalocyanine COFs, CoPc-Ph-COF and CoPc-3Ph-COF, were successfully synthesized by nucleophilic substitution reactions of cobalt (II) hexafluorophthalocyanine ($CoPcF_{16}$) with 1,2,4,5-tetrahydroxybenzene and 9,10-dimethyl-2,3,6,7-tetrahydroxyanthracene, respectively. The crystalline porous structure of these two COFs was revealed through powder X-ray diffraction and electron microscopy analysis, with a pore size range of 1.6-2.4 nanometers, which is conducive to efficient ion transport.The development of nitrogen rich conjugated phthalocyanine based mesoporous COFs materials effectively improved the migration efficiency of Li^+. This work innovatively designed and synthesized two nitrogen rich mesoporous covalent organic frameworks (COFs) based on conjugated phthalocyanines, which exhibit high specific capacity, excellent rate performance, and good cycling stability in negative electrode lithium storage performance. In particular, CoPc-3Ph-COF exhibits a reversible capacity of up to 1086 mA h g^{-1} at 100 mA g^{-1}, demonstrating its promising application prospects in high-performance LIBs. At the same time, we will delve into the cycling stability and conductivity of this type of material.

Keywords : Covalent organic frameworks, electrocatalysis, oxygen reduction, density functional theory



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Delaminated alk-MXene/Co-MOF composite membranes for high-efficiency removal of Cr(VI) and Tetracycline

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A composite membrane was designed by in-situ growth of leaf-like Co-MOF nanoparticles on the surface of alkalized MXene (alk-MXene) nanosheets. The alk-MXene/Co-MOF composite membrane with a special intercalation structure exhibits superior adsorption capacity for Chromium(VI) (Cr(VI)) and Tetracycline (TC). Herein, the embedding of leaf-like Co-MOF particles into the interlamination of alk-MXene nanosheets can promote the formation of the nanochannels, adjust the thickness of the composite membrane, and then improve its water permeability. Sample D-C2-M owns the highest pure water permeability of 443.7 L m^{-2} h^{-1} bar^{-1} and more than 98% removal rate for the pollutants with various concentrations of 10, 30 and 50 mg L^{-1}. Continuous flow dynamic adsorption test indicates that the breakthrough volume and the saturation volume of the D-C2-M composite membrane are up to 400 mL and 4900 mL, 1400 mL and 6400 mL for 100 mg L^{-1} Cr(VI) and TC solution, respectively. After 10 adsorption-desorption cycles, the removal rate of D-C2-M for Cr(VI) and TC maintains still over 95%. The superior separation capacity of the alk-MXene/Co-MOF membrane is mainly ascribed to the synergistic contributions of electrostatic interaction, hydrogen bonding, and π-π accumulation. In comparison to Cr(VI), DFT calculation verifies the preferential separation of TC from aqueous water by the composite membrane. This work provides an effective route to obtain high-performance MXene-based composite membrane with potential application prospects.

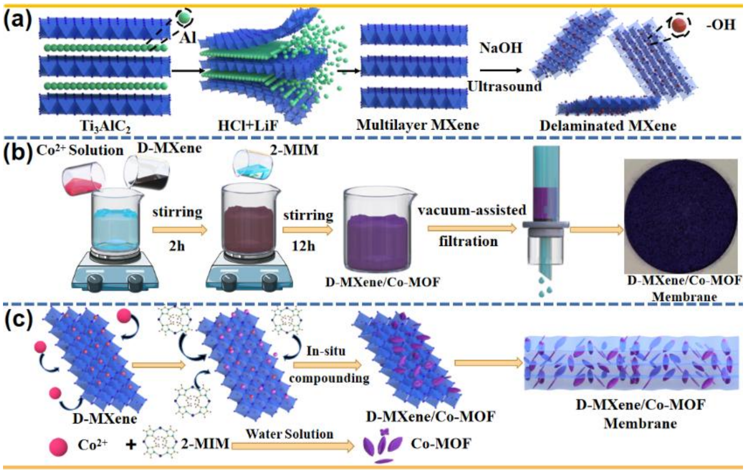

Fig. 1. Schematic preparation process of (a) D-MXene; (b-c) D-MXene/Co-MOF membranes.

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Dirac metals for two-dimensional MoS_2 semiconductors as excellent electrode

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Layered van der Waals (vdW) two-dimensional (2D) materials offer not only an excellent research platform for investigating unique quantum phenomena but also various applications to multifunctional devices thanks to their excellent physical properties, such as layer-number-dependent unique characteristics and a wide tunability appropriate for other counterpart materials. Presently vdW semiconducting 2H-MoS_2 is one of the most promising candidates among 2D materials for the future integrated circuit devices. However, a large contact resistance associated with a high Schottky barrier height and various types of disorders/defects, existing at the interfaces between a metal electrode and a semiconductor surface (M-S contact) of MoS_2, have so far been serious problems and greatly limited the ultimate performances expected in FET devices [1].

Dirac semimetal in bulk to a semiconductor in monolayer, excellent electrical conductance, large spin Hall conductance, abundant optical characteristics, and splendid thermal robustness in air have been recently reported. The seamless lateral $PtTe_2$−MoS_2 junction, created using a chemical vapor deposition (CVD), well demonstrated low contact resistance at the interface, leading to large improvements in device performances. Theoretical calculations show that the strong covalent-like interlayer coupling exists at the interface between $PtTe_2$ and MoS_2, possibly eliminating the Fermi-level pinning so that a good vdW interface contact can be made. Such a flat and smooth interface between a vdW layered metal and a 2D-vdW semiconductor could promote efficient carrier transport in contrast to the conventional ones.

In this study, we employ highly conductive Dirac metal of 1T-$PtTe_2$ in the form of a top contact for 2H-MoS_2 FETs. We exhibit that $PtTe_2$ electrodes transferred nondestructively on top of MoS_2 result in a nearly perfect metal−semiconductor interface, leading to an almost zero Schottky barrier, low contact resistance (1.58 $K\Omega\cdot\mu$m), and other superior device performances such as high mobility reaching 85 $cm^2\ V^{-1}\ s^{-1}$ at 200 K and a good on/off current ratio of over showing a large dynamic range in comparison to those of other reported electrodes [2]. Detailed discussions and interpretations, due to highly efficient FET performances of 2H-MoS_2 with 1T-$PtTe_2$ electrodes, are presented by comparing various electrodes from the viewpoint of work functions including the Dirac semimetal of graphene. Our studies contribute to the advancements in the performance of MoS_2 FETs and provide a future route to 2D-vdW materials toward the realization of a flawless M−S interface with the quantum limit.

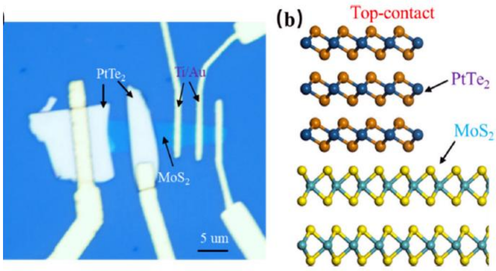

Fig. (a) Structure in 2H-MoS_2 FETs with top-contact Dirac semimetal 1T-$PtTe_2$ electrodes. Both Ti/Au and $PtTe_2$ electrodes in MoS_2 FETs on the same semiconducting MoS_2 flakes are fabricated and are subjected to accurate studies. (b) Schematic pictures of top-contact Dirac semimetal 1T-$PtTe_2$ and 2H-MoS_2 semiconductors.

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Intimately mixed copper, cobalt, and iron fluorides resulting from the insertion of fluorine into a LDH template

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Our research focuses on developing a new class of cathodes for lithium-ion batteries using fluorinated multimetallic materials. These cathodes are based on a mixture of CuF_2 and FeF_3, obtained through an innovative Multimetallic Template Fluorination (MMTF) method, using a layered double hydroxide (LDH) as a precursor $[M_{1-x}^{2+}M_x^{3+}(OH)_2]\cdot A_{x/n}^{n-}\cdot mH_2O$ [1]. We synthesized various LDH compositions via co-precipitation to assess Cu^{2+} and Fe^{3+} incorporation.

X-ray diffraction (XRD) data enabled the construction of a ternary (Mg-Co-Cu) diagram (Figure 1) to optimize the divalent composition while maintaining a constant trivalent fraction $(Fe_{0.5}Al_{0.5})^{3+}$. This diagram highlights the absence of an LDH structure in high-copper-content regions due to the Jahn-Teller effect.

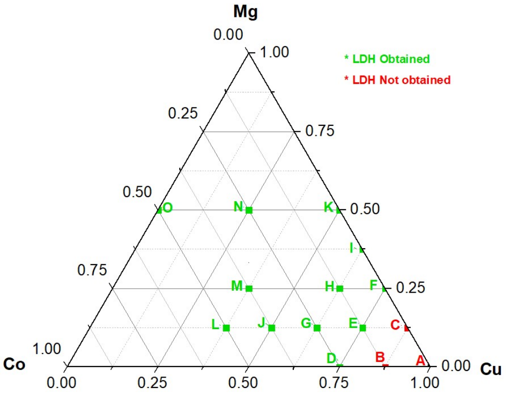

Figure 1 : Various compositions tested for different divalent metal ratios in a ternary Cu-Mg-Co diagram, representing points such as (A): $(Cu_2)^{2+}$ $(Fe_{0.5}\,Al_{0.5})^{3+}$, (B): $(Cu_{1.75}\,Co_{0.25})^{2+}$ $(Fe_{0.5}\,Al_{0.5})^{3+}$, (C): $(Cu_{1.75}\,Mg_{0.25})^{2+}(Fe_{0.5}\,Al_{0.5})^{3+}$

Among the wide range of synthesized materials, two theoretical compositions were selected for fluorination and electrochemical testing: **CCFA**: $[(Cu_{1.5}Co_{0.5})^{2+}(Al_{0.25}Fe_{0.75})^{3+}(OH)_6]\cdot(Cl^-)_1\cdot mH_2O$ and **CCF**: $[(Cu_1Co_1)^{2+}(Fe_1)^{3+}(OH)_6]\cdot(Cl^-)_1\cdot mH_2O$.

These compounds were fluorinated using the MMTF method at different temperatures (200, 350, and 500 °C). Various analyses were performed, including X-ray diffraction, Mössbauer spectroscopy, and scanning electron microscopy. This presentation will cover the development of these materials, from synthesis to electrochemical testing, highlighting the characterization phase and the transformation mechanism of LDH into metal fluorides (MF_x).

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Superconductivity of alkali C_{60} fullerides viewed from electrical conductivity

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Many high-T_c materials emerge in systems with strong on-site Coulomb repulsion (Hubbard U), where spin fluctuations from electron-electron (e-e) interactions are believed to play a central role. A diverse range of high-T_c new superconductors challenges the conventional Bardeen-Cooper-Schrieffer (BCS) framework, which attributes the formation of Cooper pairs solely via electron-phonon (e-ph) interactions. Recent studies suggest that both e-ph and e-e interactions are comparably significant in realizing high-T_c superconductivity. Alkali-doped C_{60} fullerides (A_3C_{60}, where A = K, Rb, Cs) provide a unique platform for investigating unconventional superconductivity. These systems exhibit the highest T_c among molecular superconductors at 33 K at ambient pressure [1] and 38 K under high pressure [2]. In A_3C_{60} fullerides, electron correlations are believed to play a crucial role in addition to e-ph interactions, distinguishing them from other high-T_c superconductors. Moreover, the superconductivity in A_3C_{60} is governed by a three-orbital Hubbard model arising from triply degenerate t_{1u} orbitals derived from carbon s and p states. $Rb_xCs_{3-x}C_{60}$ fullerides with expanded unit cell volumes (V_{cell}) residing in the Mott insulator (M-I) boundary are a key family for understanding the superconducting mechanism. However, significant conclusions have largely been drawn only from magnetic and vibrational studies, with limited attention to electrical transport. Here, we report systematic experiments on electrical transport σ (T, x, P) at ambient and under high pressure [3,4]. Our work significantly fills a void in understanding the mechanism of superconductivity of alkali A_3C_{60} fullerides. This provides a crucial advantage in gaining an intrinsic understanding of the superconducting mechanism of this family of superconductors.

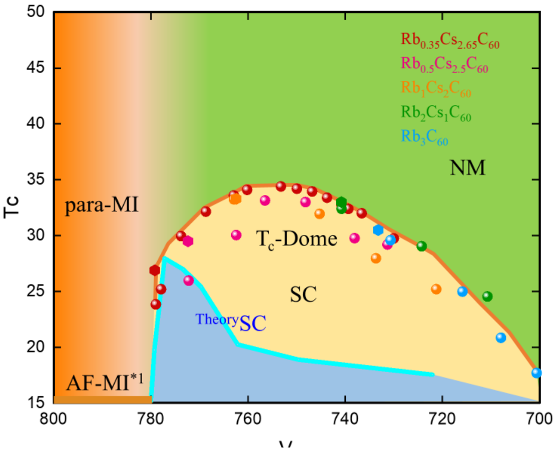

Fig. Superconducting dome of A_3C_{60} fullerides made on electrical transport data

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New ways to intercalate corrosion hydroxyquinoline-based inhibitor molecules in LDH : paradigm changes in synthesis protocols

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Recently, the most widely adopted method for protecting metallic substrates against corrosion is the application of protective coatings. Once corrosion has initiated, the polymer coating loses its ability to protect the damaged area, and it becomes essential to incorporate self-healing capabilities into coatings specifically, the ability to autonomously repair defects and provide long-term protection [1]. Chromate-based systems are known for their active corrosion inhibition properties, yet their use is being phased out due to their high toxicity and carcinogenicity. Thus, it is imperative to create new systems with self-repairing functions as alternatives to chromate-based solutions. The 8-hydroxyquinoline (HQ) molecule has already been the purpose of numerous works due to a broad range of applications such as metal cations detection and removal, organic light emitting diodes and medicine. Corrosion inhibition efficiency of HQ has also been studied as it could be an environment-friendly candidate for the replacement of chromates for aluminium-based alloys [2]. All of these uses are based on the ability of the quinoline based-compounds to complex metal ions and to be detected by UV/visible or fluorescence. One of the most studied derivatives of HQ was the 8-hydroxyquinoline-5-sulfonic acid (HQS). However, direct incorporation of inhibitory species into coatings may lead to detrimental interactions between the matrix and the active species, resulting in a loss of inhibitory performance degradation of the coating. A promising approach to circumvent this issue is the encapsulation of inhibitors within host structures. These materials can store inhibitors while preserving the protective properties of the coating. When the protective properties are compromised, the active species are released to inhibit further corrosion. Layered double hydroxides (LDHs) are promising cargo materials for this purpose [3], as they can incorporate anion corrosion-inhibiting molecules. As anion exchange host, LDHs structure converts into organic inorganic hybrid material by the incorporation of the organic molecule. Studies relating the intercalation of HQS in LDH is scarcely reported as it appears challenging to form such hybrid material due to the molecule rapid complexation with metal cations, thus preventing any syntheses by usual coprecipitation or exchange protocol [4]. We propose here to focus on the intercalation of 8-HQS, adopting a change of paradigm from the classical anion exchange reactions since rather low exchange rate, pH unstable for the host and associated to short contact times are optimized.

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Preparation of Layered Double Hydroxides with Varied Layer Charge

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Layered double hydroxides (LDHs) are a large class of two-dimensional materials which is represented by a general formula $[M_{1-x}^{II}M_x^{III}(OH)_2]^{x+}[A_x^{m-}\cdot nH_2O]$, encompassing a variety of metal (M^{II} and M^{III}) and anion A. The tunability of composition and consequently physical/chemical properties of LDHs critically depend on the degree of substitution of M^{III} into the brucite-like layer $M^{II}(OH)_2$, via $x = (M^{III}/(M^{II}+M^{III})$. Accordingly, a rational design of low-charge density LDH was reported, showcasing three important criteria: (i) close ionic radii of M^{II} and M^{III}, (ii) bulky interlayer anion (e.g., dioctyl sulfosuccinate), and (iii) incorporation of large molecules for the possible interlayer solvation (e.g., glycerol). Taking NiFe-LDH as an example, the difference in ionic radii between Ni^{II} and Fe^{III} is ~6%, which is very small compared to other $M^{II}M^{III}$ combination(e.g., 28% for ZnAl-LDH and 26% for MgAl-LDH). Following these guidelines, we have prepared a single-phase NiFe-LDH with exceptionally low x = 0.04-0.05 (CD = 0.31 nm^{-2}). It showed enhanced adsorption capacity toward Cr^{VI} relative to the higher CD analog (x = 0.30).[4] Single phase NiFe-layered double hydroxides (LDH) with low and high charge densities (CD, 0.85 vs 3.23 nm^{-2}; $Fe^{III}/(Ni^{II} + Fe^{III})$ = 0.05 and 0.25) were successfully prepared by the coprecipitation in aqueous glycerol using urea under hydrothermal conditions. The low-CD NiFe-LDH showed decreased apparent activation energies of water evaporation and of glycerol decomposition, suggesting diminished intercalates/layers interactions relative to the high-CD one, which was evidenced by the electric conductivity.[5] The hybridization of LDHs with other solid components is another approach to design functional materials, where controlled CD can play positive roles.

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Anomalously large thermoelectric Seebeck observed in intrinsic organic semiconductors

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The Seebeck effect is the thermoelectric conversion of a temperature difference into an electric voltage in materials. The values of Seebeck are generally known to be in the μV/K scale, ranging from 1 to 500 μV/K in various materials. The Seebeck values of typical metals or deeply doped semiconductors are less than k_B/e (~ 86.25 μV/K), while those of lightly doped or intrinsic semiconductors are larger but less than 500 μV/K [1]. Numerous studies so far demonstrated that the Seebeck values of some organic semiconductors reach a value of 1000 μV/K [2]. These results are attributed to the disorder present in the materials, and an explanation was given based on the Heikes formula [2]. In recent years, however, some intrinsic organic semiconductors have been reported to exhibit an extremely large Seebeck value (so-called Giant Seebeck: GSE), reaching a value of 10 mV/K and attracting considerable attention [3]. Currently, the intrinsic mechanism of such GSE has not been unveiled. We focus on the GSE of intrinsic organic semiconductors by targeting rubrene single crystals [4,5]. We provide firm experimental confirmation by direct measurements, employing a differential amplifier equipped with a tera-ohm high resistance. GSE exceeding 6 mV/K was observed in both the hole and electron carrier regimes when a field effect transistor technique was applied. In the framework of the semiclassical description of Boltzmann transport equations of thermoelectric transport, we interpret the GSE in terms of the existence of impurity bands and the lower mobility at the band edge.

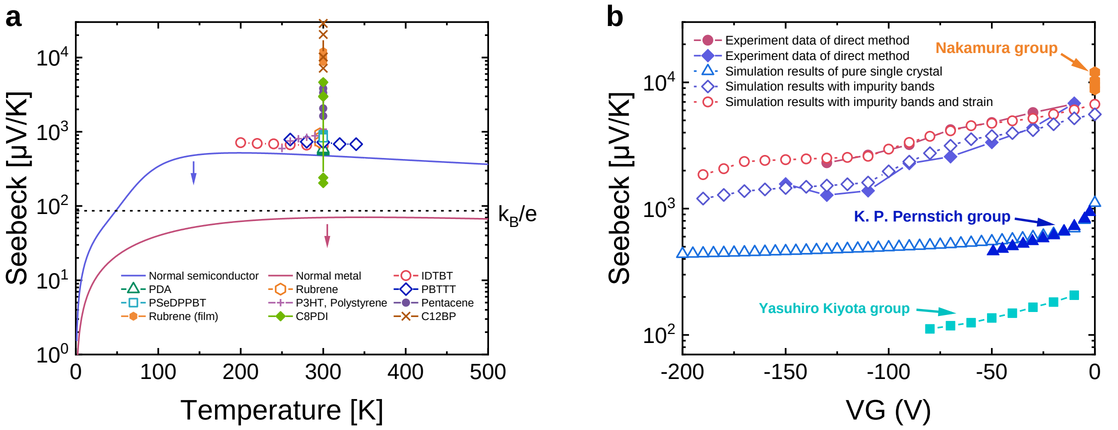

Fig. a. Seebeck values of various materials as a function of temperature; **b**. Experimental data and theoretical simulations of the GSE in rubrene single crystal.

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Visualizing Atomic Quantum Defects in Ultrathin 1T-PtTe$_2$

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Defects are significant to determine and improve the distinct properties of 2D materials, such as electronic, optical, and catalytic performance. We observe four types of point defects in atomically thin flakes of 1T-PtTe$_2$ by using low-temperature scanning tunnelling microscopy and spectroscopy (STM/S). Through the combination of STM imaging and simulations, such defects are identified as a single tellurium vacancy from each side of the top PtTe$_2$ layer and a single platinum vacancy from the topmost and next layer. Density functional theory (DFT) calculations reveal that the platinum vacancies from both the monolayer and bilayer exhibit local magnetic moment. In bilayer PtTe$_2$, the interlayer coulomb screening effect reduces the local magnetic momentum of the single platinum vacancy. Our research provides meaningful guidance for further experiments about the effects of intrinsic defects on the potential functions of thin 1T-PtTe$_2$, such as catalysis and spintronic applications.

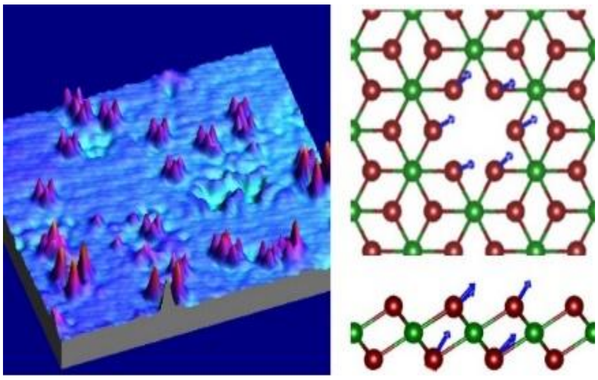

Fig. 1 The STM image and atomic structure of the defective PtTe$_2$

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Micron-Scale antioxidant Intercalated layered double hydroxides for enhanced gas barrier and thermal stability in polyurethane composites

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As the fifth largest plastic, polyurethane (PU) has excellent mechanical properties, stability, wear resistance, etc., and is one of the most suitable polymer materials as a gas barrier material. However, due to the low atomic packing density of the polymer itself, there are still challenges to improve its gas barrier performance in food packaging, hot air balloons, airships and other fields[1]. The gas barrier properties can be improved by adding sheet nano-reinforced phase such as graphene and montmorillonite to the polymer[2]. However, the traditional filler treatment process is more complicated, which limits the application of PU.

As a two-dimensional anionic layered material with adjustable interlayer anions, layered double hydroxide is more flexible than traditional fillers, and is a better choice to improve the gas barrier performance of PU. In this work, macromolecular anionic antioxidants were introduced into the interlayer to expand the layer spacing and improve the dispersion of inorganic fillers in the polymer, enhance the gas barrier property of the polymer, and optimize its oxidation resistance to a certain extent. We successfully prepared a series of large-scale micron antioxidant intercalation layered double hydroxide D-LDH using a combined strategy of hydrothermal and ion exchange, and by precisely controlling the concentration of metal Mg^{2+} in hydrothermal synthesis, which improved the gas barrier properties of PU composites. Among them, 0.2-D-LDH/PU (5 wt%) showed optimal gas barrier performance and thermal stability. The addition of antioxidants promoted the crystallization of PU by heterogeneous nucleation, and enhanced the hydrogen bond interaction between the hydroxyl group on the layered double hydroxide and the polymer, which improved the mechanical properties of the composite. There is no doubt that micron D-LDH, as a two-dimensional layered material, has excellent gas barrier properties, while improving the thermal stability and mechanical properties of composite materials, and has practical application value.

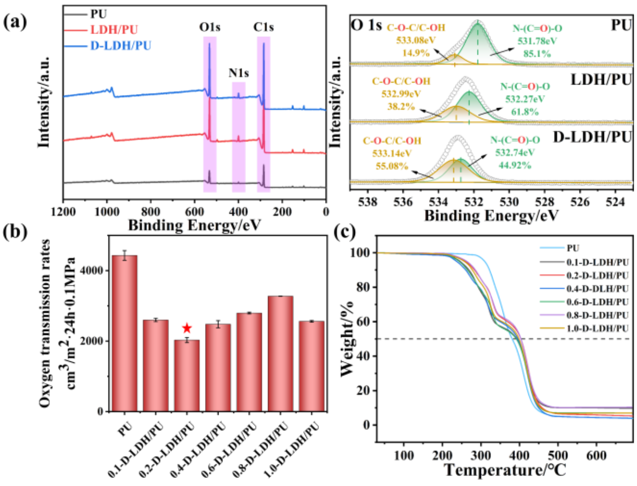

Figure 1. (a) XPS spectra of PU、LDH/PU、D-LDH/PU; (b) Oxygen transmission rates (OTR) and (c) Thermogravimetry Analysis (TG) of n-D-LDH/PU.

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Innovative soft chemistry approach for cation insertion in layered perovskite oxides: chemical and multi-technique structural investigation

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The development of multifunctional layered hybrid materials extends across various research domains. Among these, layered perovskites (Aurivillius (AV), Dion-Jacobson (DJ), Ruddlesden-Popper (RP) type) are particularly promising, as their functionalization with organic compounds is well established.[1–4] Recently, our team demonstrated the possibility of inserting metallic cations within these phases, broadening their potential applications. Since this approach remains relatively unexplored, it is essential to investigate the experimental conditions for insertion and conduct a structural analysis to better characterize and understand the resulting material.

This presentation will demonstrate the possibility to insert a wide range of metallic cations into layered perovskites using an innovative approach. As an example, a multi-emission behaviour resulting from the insertion of rare earth element will be presented. Subsequently, a structural investigation will be presented, using the example of copper insertion into the DJ phase $RbLaNb_2O_7$ and the AV phase $Bi_2SrTa_2O_9$, where the latter results in a 1 eV reduction in the material's band gap. To achieve this, various characterization techniques have been employed, including spectroscopic methods such as X-ray Absorption Spectroscopy (XAS), Electron Paramagnetic Resonance (EPR), and Electron Energy Loss Spectroscopy (EELS), which provide insights into the local environment of the inserted cations thus enabling the correlation between the obtained properties and the deduced structural models.

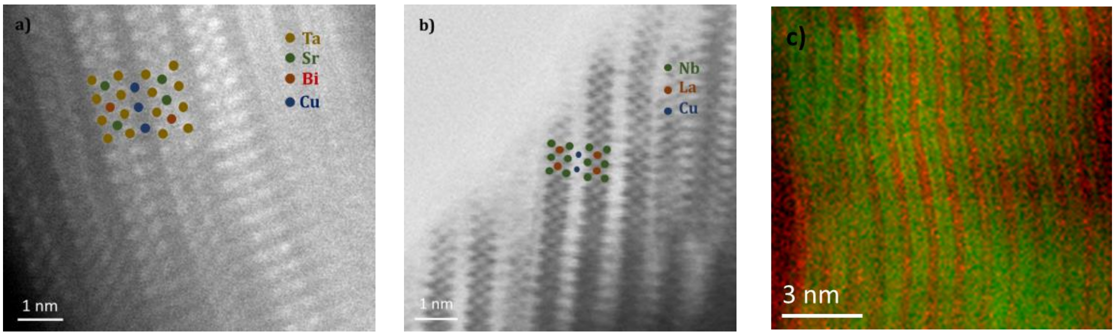

Figure: HRTEM images of copper inserted in a) $Bi_{0.1}Sr_{0.85}Ta_2O_7$ layers, b) $LaNb_2O_7$ layers, c) EELS mapping of copper (red) superimposed on the starting HAADF image (green)

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Dual-Metal-Substituted Ruthenate Perovskite Oxide for Efficient Alkaline Hydrogen Evolution

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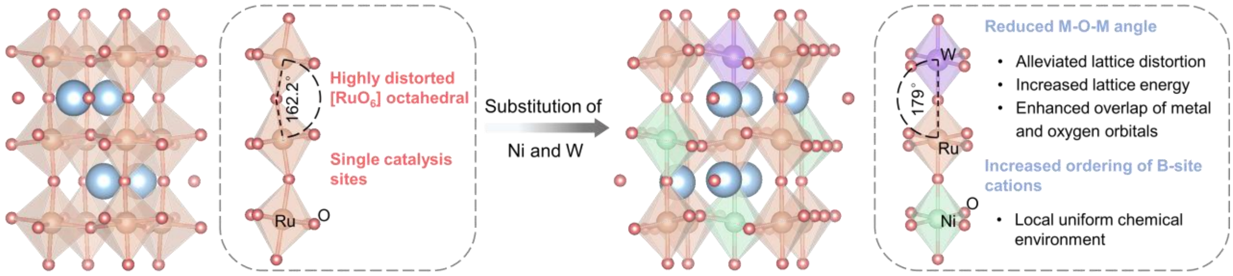
Identifying and regulating catalytically active sites are essential for developing efficient electrocatalysts for alkaline hydrogen evolution reaction (HER) and deepening the fundamental understanding of operation mechanisms. Herein, we introduce a dual-element gradient-valence doping strategy (DSGS) to incorporate elements with significant valence state difference into the B-sites of $SrRuO_3$. This valence difference induces the ordered arrangement of multiple active sites and creates chemically uniform local environments, making the catalyst suitable as a platform catalyst for investigating the reaction mechanism. More importantly, the electronic structure of active sites can be precisely controlled by varying the type and concentration of dopants. The perovskite with optimal chemical composition, i.e., $SrRu_{0.6}Ni_{0.3}W_{0.1}O_3$ catalyst, achieves an ultralow overpotential of 44 mV at 10 mA cm^{-2} and exceptional durability exceeding 500 hours, setting a new benchmark for alkaline HER performance. Combined X-ray photoelectron spectroscopy and X-ray absorption spectroscopy reveal that the Ru species are oxidized to a higher valence state via an efficient electron transfer from Ru sites to neighbouring metal sites. The *in-situ* spectroscopy reveals that these dopants modulate the electronic structure of Ru active centers and stabilize reaction intermediates that migrate via hydrogen spillover effect. Additionally, the formation of oxygen vacancies in the host lattice helps reduce the energy barrier for water adsorption. These findings underscore that a new descriptor–the synergy between B–O covalency and oxygen vacancies–that enhances water activation and enables elastic valence changes of active sites. This study offers a universal framework for designing high-performance alkaline HER catalysts and advancing mechanistic understanding in sustainable hydrogen production.



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Screening the potential of Prussian blue analogues for novel proton batteries

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In the field of stationary energy storage, aqueous batteries offer a safer and lower-cost alternative to organic batteries, with aqueous proton batteries (APBs) emerging as a promising alkaline-free option. While several families of materials for APBs have been identified[1,2], Prussian blue analogues (PBAs) exhibit interesting performances notably thanks to their unique proton conduction properties. Wu et al.[3] attributed the extremely high rate capability of a water-rich Cu-based PBA cycled in 2M H_2SO_4 to a Grotthuss mechanism—the coordinated transfer of H^+ along a chain of (crystal) water molecules. Synthesis conditions of PBAs make it possible to control the crystal water content through the amount of vacancies, as reflected in their general formula: $A_xM_A[M_B(CN)_6)]_y\square_{1-y} \bullet zH_2O$ (A is the insertion ion, M_A and M_B elements from the d or p-block). To better understand structure-performance relationships, we synthesized a large range of PBAs with varying water content via a simple co-precipitation method with M_A=V, Mn, Fe, Co, Ni, Cu, Zn, Al, Sn and M_B=Fe. The materials were finely characterized via XRD, ICP, TGA, and Mössbauer spectroscopy. Electrochemical testing in 4.5M acetic acid (a weak acid) led to promising performances for Zn, Cu or V based materials. The iron redox potential is shown to depend on the nature of the second transition metal, offering an adaptability to the electrolyte's electrochemical window. Hydrated PBAs exhibited reduced polarization, supporting the role of crystal water in proton diffusion. Paradoxically, the non-hydrated Zn-PBA showed the best performance, with a plateau at 1.07V (vs SHE) and 74mAh/g capacity as shown in Fig 1. This behaviour suggests that the Grotthuss mechanism solely cannot explain proton insertion/diffusion in these materials. EQCM experiments should allow to clarify the processes involved.

Top-performing PBAs were also tested in Protic Ionic Liquids such as pyrrolidinium acetate to widen the potential window, and increase the energy density. Addition of dry acetic acid into the IL electrolyte improves significantly the electrochemical behaviour (Figure 2).

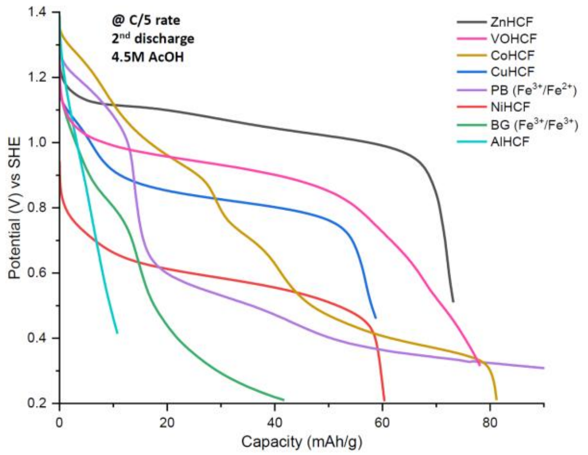

Figure 1 : *2nd discharge of PBA materials at C/5 rate in 4.5M acetic acid*

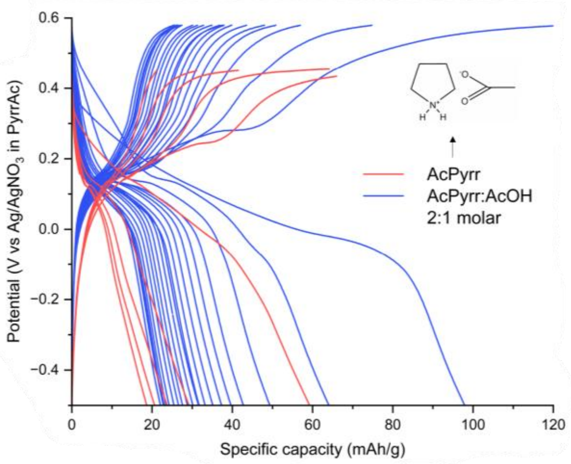

Figure 2 : *C/10 cycling of an hydrated Cu-PBA either in pure pyrrolidinium acetate or mixed with acetic acid*

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Solar hydrogen production under the Caribbean sun

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The θ phase of the layered nanomaterial zirconium phosphate ($Zr(HPO_4)_2 \cdot 6H_2O$, θ-ZrP) can be directly ion-exchanged with electrocatalysts, producing intercalated phases useful for water splitting applications. Electrocatalysts for the oxygen evolution reaction (OER) have been incorporated within ZrP as intercalated species, or surface bound, on exfoliated layers, and on nanoparticles of different morphologies (hexagonal platelets, cubes, rods, and spheres). Single and bimetallic electrocatalysts based on earth-abundant materials have been studied. Reduction in overpotentials and increases in mass activity have been achieved. Mixed metal NiFe-intercalated ZrP electrocatalysts at 90% Fe metal content proved to have superior OER electrocatalytic performance (decreased overpotentials, increased mass activities, reduced Tafel slopes) compared to adsorbed counterparts. We are exploring OER activities of other mixed-metal catalysts on ZrP, bifunctional catalysts, and operando synchrotron XAS studies to elucidate the nature of the active species. Recently we have prepared CoFe electrocatalysts systems supported on ZrP. Preliminary results with the CoFe electrocatalyst system show that the intercalated bimetallic system is more active than the surface-adsorbed one as evidence by the lower overpotential. Previous EXAFS operando studies conducted at CHESS provide possible models of a Co electroactive site. Apart from working with Co, Fe, and Ni-based electrocatalysts and their mixed systems, we are also working on Mn-based electrocatalysts. We are exploring OER activities of these new mixed-metal catalysts on ZrP, studying if these catalyst systems can also be bifunctional catalysts (if they also show activity for ORR or HER), and conducting operando synchrotron XAS studies to elucidate the nature of the electrocatalytic active species. We are also exploring efficient solar H production using these supports by incorporating photoadsorbers in photoelectrochemical cells.

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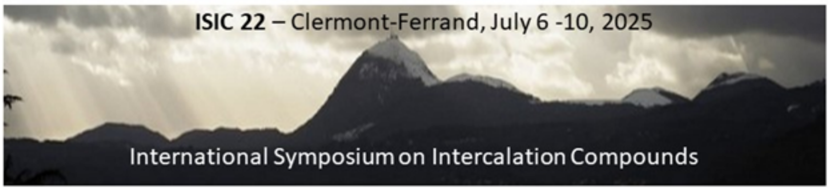

Layered Double Hydroxides as Hosts for Controlled Nutrient Release in Sustainable Agriculture

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The need for sustainable agricultural practices has intensified due to the growing global demand for food and the environmental impact of conventional fertilization strategies.[1,2] Excessive reliance on soluble chemical fertilizers contributes to nutrient leaching, soil degradation, and greenhouse gas emissions, necessitating innovative approaches to improve nutrient use efficiency.[3] One promising strategy involves intercalation compounds capable of controlled nutrient release, ensuring better synchronization with plant uptake while mitigating environmental losses.[1]

In this study, we explore the potential of layered double hydroxides (LDHs), as host structures, for nutrient storage and gradual release in agricultural soils. LDHs, with their unique anionic exchange capacity, are enriched with essential plant nutrients and incorporated into biochar matrices to enhance stability and performance.

LDHs were synthesized via co-precipitation, enriched with essential plant nutrients through ion exchange or direct intercalation, and then integrated into biochar matrices. Release kinetics were initially assessed in batch systems to determine short-term nutrient availability, followed by soil column experiments to evaluate leaching behaviour under conditions that mimic agricultural environments. The results indicate that incorporating LDHs within biochar matrices was particularly advantageous in the column experiments, where the biochar-LDH composite released more nutrients over 72 hours than the nutrient-enriched biochar alone. These findings highlight the potential of LDH-based fertilizers to enhance nutrient availability and retention, contributing to more efficient and environmentally sustainable fertilization practices.

Acknowledgments:

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Defect and Interface Engineering in Two-Dimensional Inorganic Nanosheet-Based Electrocatalysts

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The defect engineering of nanostructured materials has garnered significant research interest due to its utility in exploring high-performance energy-functional materials. The introduction of crystal vacancies into nanostructured material is found to be quite effective not only in tailoring the electronic and local structures but also in increasing the electrochemical activity. Since crystal defects can serve as efficient adsorption/reaction sites for ions, electrolytes, and catalysis reactants, the defect engineering can provide a versatile means to optimize the electrocatalyst functionalities of nanostructured materials. In this talk, I will present diverse examples of defect-engineered nanostructures along with the correlation between chemical bonding nature and energy functionalities. The various roles of crystal vacancies in optimizing the catalyst performances will be highlighted based on combined in situ/ex situ spectroscopic analyses.

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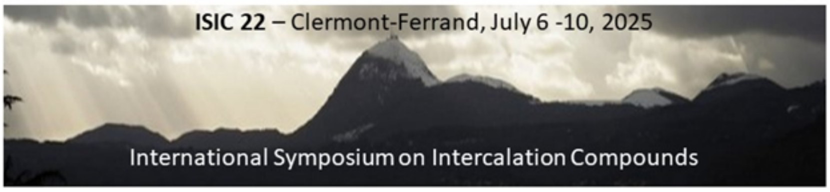

Different porous adsorbents for PFAS removal from aqueous solutions

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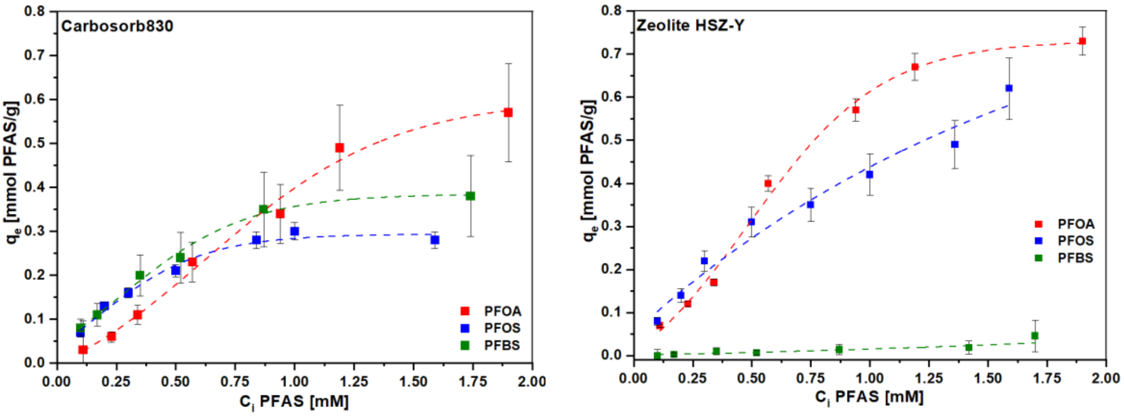
Fluorinated alkyl substances (PFAS) are a class of amphiphilic organic molecules that differ in alkyl carbon chain length and polar functional group at the head of the chain. Since their carbon chain is fully fluorinated, they are very stable and persistent, exhibiting both hydrophobic and lipophobic properties. The presence of some PFAS in aquatic environment is of great concern as toxicological data suggests an association with adverse human health effects [1]. Here, a commercial granular activated carbon (Carbosorb830) and an ultra-stable high-silica Y zeolite were used as adsorbents for the removal of three PFAS molecules from water within a concentration range between 50 and 800 ppm. Perfluorooctanoic acid (PFOA), perfluorooctanesulfonic acid (PFOS) and perfluorobutanesulfonic acid (PFBS) were used as model PFAs molecules. ^{19}F-NMR spectroscopy was used for the identification and quantification of PFAS. In Figure 1 the adsorption curves representing adsorption experiments performed at different PFAS concentrations are reported. It is observed that zeolite Y exhibits a higher adsorptive capacity for PFOA and PFOS compared to commercial carbon. Adsorption capacities above 0.7 mmol/g for PFOA and 0.6 mmol/g for PFOS were found when Y zeolite was put in contact with pollutants concentrations above 1.75 mM. However, an extremely low adsorption has been found for PFBS. Carbosorb830 however has been able to also adsorbed up to 0.4 mmol/g of PFBS for concentration around 1.75 mM. For PFOA the adsorption capacity was slightly lower than that of Y zeolite reaching 0.6 mmol for concentrations around 2 mM. PFOS however was adsorbed by Carbosorb830 in lower quantities with respect to Y zeolite, around 0.3 mmol/g. To verify the behaviour of adsorbent materials in the presence of two PFAS compounds, adsorption of binary solutions (PFOA/PFOS and PFBS/PFOS) were tested. Finally, solid-state NMR spectroscopy experiments were conducted on the materials after adsorption to gain additional information on adsorbent/adsorbate interactions. Close contact between PFAS molecules and the surface of Y zeolite was observed through the appearance of the Si signal associated with the zeolite structure thanks to the cross polarization process between ^{29}Si and ^{19}F.



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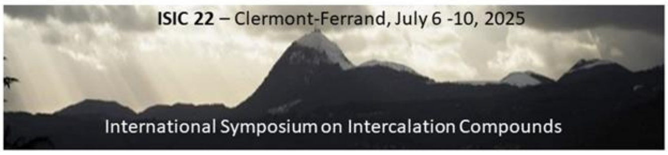

PoLA (Porosity Local Analysis): An Accurate Descriptor of Microporous Volume to Predict Gas Adsorption in Porous Carbons

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A procedure is presented to describe the porosity of microporous solids (e.g. activated carbons): unlike many methods commonly used at present, PoLA (Porosity Local Analysis) is not based on pre-defined pores of regular shape (like spheres or cylinders) but rather on a point-by-point analysis of the inner voids.

Then PoLA is particularly suited to describe amorphous porous materials, like activated carbons, accurately: the procedure can be applied to any atomistic model and it is much faster than other methods in wide use (as for instance the popular PoreBlazer tool). More important, the porous volume distribution provided by PoLA is strongly correlated to gas adsorption isotherms and it can be used to predict the adsorption in new materials effectively.

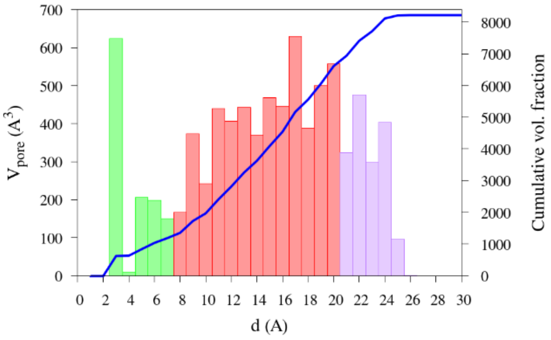

Figure 1: A typical distribution of the porous volume as provided by PoLA. Green: ultramicroporous, red: microporous; purple: mesoporous fraction; blue: cumulative porous volume.

We proved this point by preparing a large dataset of porous carbon models which were analyzed by PoLA; accurate N2 adsorption isotherms at 77 K were simulated with Grand Canonical Monte Carlo in each model system, and the isotherms were correlated to the porosity distribution by a machine learning (Random Forest) approach. The multiple regression parameters were then used to predict the isotherms in various carbon models, with excellent results.

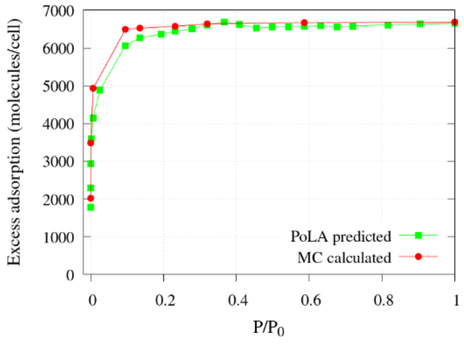

Figure 2: N_2 at 77 K adsorption isotherm in a large carbon model, computed by high level GCMC and predicted on the basis of PoLA porous volume distribution.

On this basis, PoLA can also be used to deduce the porous volume distribution from experimental nitrogen or argon adsorption isotherms and then predict the performance towards other gases of interest, like hydrogen, methane or carbon dioxide.

Single-component and binary H_2O and CO_2 co-adsorption isotherm model on amine-functionalised Mg-Al mixed metal oxides

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H_2O is a ubiquitous component of ambient air, and its content (0.5–3%) is much higher than that of CO_2 (approximately 400 ppm). Despite their high affinity for CO_2, amine-functionalised porous materials adsorb significant amounts of H_2O because of the hydrophilic nature of amine groups. Studies have confirmed that H_2O plays a complex role in DAC [1, 2, 3]. The presence of H_2O significantly affects the CO_2 adsorption mechanism of amine-functionalised adsorbents, leading to changes in their CO_2 adsorption capacity, long-term stability, and kinetics.

One challenge is that most of the studies reviewed above only discuss qualitative observations. Accurate H_2O and CO_2 co-adsorption models for amine-functionalised sorbents are lacking. Owing to the strong affinity between the amine group and H_2O, additional energy is required for the regeneration of desorbed H_2O [4]. Consequently, for the design and cost analysis of amine-functionalised adsorbent-based DAC systems, a detailed understanding of single-component and binary co-adsorption of H_2O and CO_2 is essential. Because few attempts have been made to systematically study the H_2O and CO_2 co-adsorption on amine-functionalised adsorbents, accurate estimation and optimisation of the energy consumption of the DAC process have been hindered.

The coupled thermodynamic-diffusion kinetic regulation of CO_2 adsorption by hydrothermal synergy is the key to optimizing the DAC process. Based on the amine-functionalised layered double hydroxides system, we constructed a theoretical model of one/two-component synergistic adsorption to reveal the mechanism of co-adsorption: the Guggenheim-Anderson-De Boer (GAB) model was used to analyze the multilayer adsorption of water vapors and the pore wetting behaviors, and the improved Sips model fused the thermodynamic equilibrium of amine-based active sites with diffusion limitations of polymer chains. The proposed mechanistic binary isotherm model reveals the nature of the water molecules to enhance the CO_2 adsorption capacity through the synergistic pathway of solvation-enhanced diffusion-amine group activation. The experimental data showed that at 0.1 mbar CO_2 partial pressure, the presence of water vapor increased the CO_2 adsorption capacity by 57% at 25 °C compared with the dry condition, and the increase was significantly expanded to 6.5-fold at 50 °C, demonstrating the temperature-driven diffusion-activation effect. The model constructs a temperature-sensitive parameter system: (1) temperature correction of the maximum adsorption capacity based on the Arrhenius equation; (2) a dynamic model of the diffusion coefficient incorporating the conformational transition of the amine-based polymer chain segments; and (3) a gradient of the competing adsorption potentials for the amine-based active sites. Validated by fixed-bed breakthrough experiments, the model has a prediction error of <8% in the range of water vapor partial pressures of 0.9-1.9 mbar and temperatures of 25-75 °C, and successfully captures the hydrothermal synergistic nonlinear features in the region of very low CO2 partial pressures (0.04-0.4 mbar). The synergistic effect was found to be weak at conventional concentrations (>1000 ppm), while showing a quadratic growth pattern at very dilute conditions. The model quantifies the adsorption competition mechanism between hydroxyl and amine active sites on the LDH surface at a theoretical level.

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In situ capture of initial nucleation particles for layered double hydroxides

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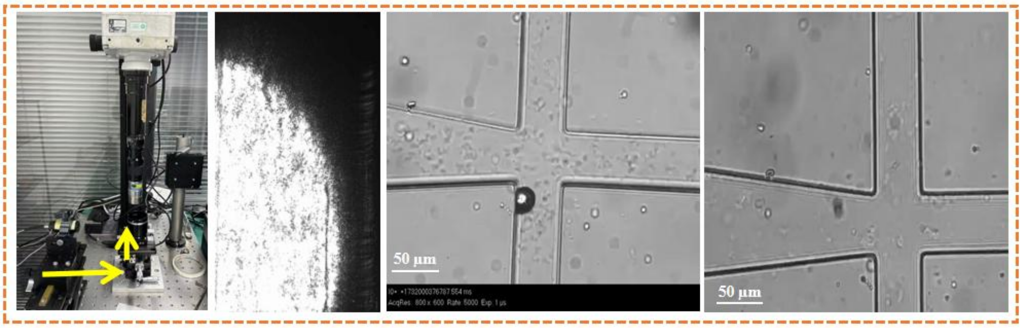
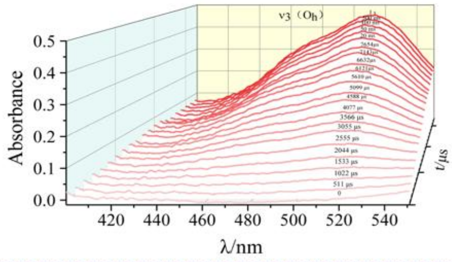
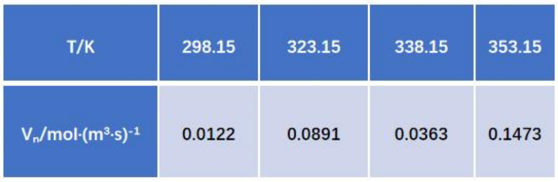
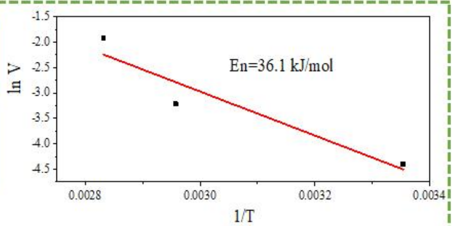
To reveal the key micro mechanisms involved in the rapid phase transformation process of inorganic functional materials such as layered double hydroxides (LDHs), a high time and spatially resolved in-situ multi characterization system for nucleation reactor was proposed involving high speed camera, microsecond level time-resolved fiber optic spectrometer, time-resolved Raman spectroscopy and nanoscale laser confocal fluorescence imaging. Based on this system, multi-dimensional and real-time multi-channel monitoring from chemical bonds to the nanoscale was achieved, and the micro mechanisms and dynamic laws of the nucleation process of inorganic functional materials such as LDHs in a rotating liquid film reactor were obtained. Based on experimental data, the nucleation kinetics, nucleation and growth models under complex flow fields were established, providing theoretical guidance for the design and development of a series of inorganic functional materials, as well as industrial large-scale preparation.







T/K	298.15	323.15	338.15	353.15
V_n/mol·(m^3·s)$^{-1}$	0.0122	0.0891	0.0363	0.1473



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Organic-inorganic hybrids having a talc-like structure as hosts for light-driven applications

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Organic-inorganic hybrids having a talc like structure (TLH) can be prepared by a process based on sol-gel chemistry which enables the formation of the materials under mild conditions in a one-step method. In this case, thanks to the use of organoalcoxysilanes as silicon sources, functional groups are covalently linked to the silicon atoms of the tetrahedral sheets and are pending in the interlayer space and present at the surface [1].

The goal of this study is to create a new type of photopolymerizable organic-inorganic hybrids talc-like structure containing photopolymerizable groups and Thioxanthone, a chromophore which has often been used as triplet sensitizers and photoinitiators of polymerization and has interesting photophysical properties [2]. These hybrid materials would be able to react with light, thus opening the way to new applications in various technological fields.

A series of TLH and TX-TLH were prepared starting from organotrialcoxysilanes having different functionalities (3-methacryloxypropyl, 3-aminopropyl, 3-glycidyloxypropyl and mixtures of two or three of them), an ethanolic solution of magnesium salts and sodium hydroxide. The key parameters governing the synthesis were finely tuned for each system. It was shown that room temperature (20°C) and short aging times lead to the formation of lamellar structures as confirmed by X-Ray diffraction. The stability of the Si-C bond and the presence of TX was proven by Fourier transformed Infrared spectroscopy. ^{13}C and ^{29}Si solid state nuclear magnetic resonance shed respectively light into the structural investigations of the attachment of pendant organic chains to the inorganic framework as well as on the integrity of TX and the degree of polycondensation of silicon species.

The determination of quantum yields and lifetimes of luminescent species enable gathering information on the influence of TX confinement on the photophysical and photochemical properties. Finally, photopolymerization was performed by using Digital Light Processing (DLP).

This set of experiments showed that TLH are versatile compounds suitable to host chromophores leading to materials showing original properties.

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Preparation of novel synthetic saponite clays from agricultural rice husk and their application for the abatement of organophosphorus pesticides

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Humanity is facing harsh challenges to become a sustainable global community by reducing its impact on the Earth's precious resources. In this prospect, the reuse of waste substances from various agrifood processing to produce materials and compounds with high intrinsic value is becoming increasingly imperative. Among these, rice husk is an excellent source of cellulose, hemicellulose, lignin, silica (~20%) and trace metals.[1] Biogenic silica can be extracted and used to replace expensive and sensitive silicon sources (i.e. fumed silica, TEOS) used in the synthesis of inorganic materials such as layered clays.[2] These bio-based materials can be exploited in various fields of application, especially in environmental remediation, e.g. for the catalytically abatement of hazardous pesticides used in agricultural crops.[3] In light of these considerations, a novel synthetic saponite clay of biogenic origin was prepared through a modified hydrothermal synthesis, using the aqueous silicate solution obtained by processing amorphous SiO_2 extracted from rice husk as the silicon source (Fig. 1). Following this, Na^+ and H^+-exchanged saponites were also prepared. All solids were thoroughly characterised using a multi-technique approach. The biogenic saponite showed micrometre-sized particles, high cation-exchange capacity (>100 meq/100 g) and significant Brønsted acidity due to high isomorphic substitution of Si(IV) by Al(III) in the tetrahedral layers. The materials were then investigated in the catalytic degradation of the anti-cholinergic organophosphorus pesticide paraoxon-ethyl, known for its neurotoxic effects on insect pests of certain crops, under mild conditions (neutral pH, T_{amb} and p_{amb}) in heterogenous phase. Tests were performed in both water and ethyl acetate (AcOEt), monitoring the reaction through different techniques. In the aqueous phase, without additional additives, the H^+-saponite was able to degrade by hydrolysis >70% of the substrate after 24 h. In AcOEt, with the addition of a fixed volume of 30% aq. H_2O_2, both H^+- and Na^+-saponites were able to completely reduce the paraoxon content after 1 and 3 h, respectively, while unmodified saponite reached >90% after 24 h (Fig. 1). Studies are currently focusing on the effect of basic and/or acidic sites in the clay obtained from rice husk on the degradation mechanism of paraoxon under the experimental conditions tested.

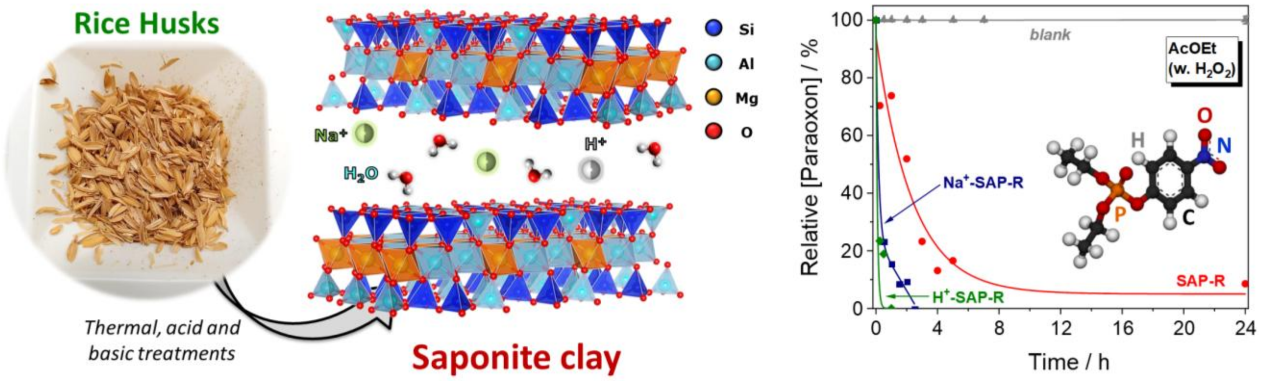

Figure 1. Abatement of paraoxon-ethyl in AcOEt with novel rice husk-derived synthetic saponite clays. Reaction conditions: 10 mL of 200 ppm (0.73 mM) pesticide solution at neutral pH, 30% aq. H_2O_2 (98 mM), 40 mg catalyst, 298 K, 1 atm, under stirring.

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Preparation and characterization of a monolithic composite composed of geopolymers and layered double hydroxides (LDH) for simultaneous immobilization of ions in an alkaline environment

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A geopolymer foam-based monolithic composite filter has been developed for the co-immobilisation of cationic and anionic pollutants. By combining geopolymer, which traps cations, with layered double hydroxides (LDH), known for their anion exchange properties, the filter enables simultaneous removal of both types of pollutants. A powder study demonstrated the synergistic effect of this combination for co-adsorption. [1] The proposed synthesis method allows the formation of monolithic filters suitable for pollutant immobilization in real case.

This work focuses on developing a geopolymer/LDH composite foam to optimize microstructure and ion exchange performance. Synthetic AFm phases (calcium-based LDH with enhanced alkaline stability) were incorporated during the alkaline activation of metakaolin-based geopolymer. Foaming, achieved using hydrogen peroxide and a surfactant, enables liquid percolation. The composites were characterized by XRD, Raman, and solid-state 27Al NMR, revealing partial carbonation and degradation of the Ca2Al-NO3 AFm phase during alkaline activation. Synthesis parameters were optimized to stabilize the composite, paving the way for co-immobilisation tests on cation/anion pairs.

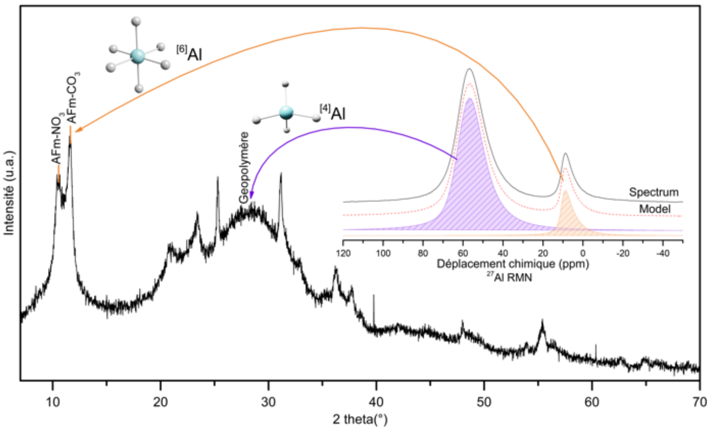

Figure 1: XRD and 27Al NMR spectra of a monolithic geopolymer/40% Ca2Al-NO3 AFm composite activated by sodium silicate, showing aluminum in tetrahedral (geopolymer) and octahedral (LDH) coordination

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Optimized Synthesis of Organic-Inorganic Hybrids having Talc-like Structure for Organic Molecules Intercalation

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Talc are naturally-occurring clay minerals made up of repetitive layers which are composed of a brucite, $Mg(OH)_2$, octahedral sheet sandwiched between two silicon oxide tetrahedral sheets. For many applications, natural talc suffers from many drawbacks such as the presence of impurities, the loss of their crystalline structure when grounded, etc. Such limitations can be overcome by employing different synthetic procedures that produce talc-like structures with modified surface properties [1]. Sol-gel process allows the synthesis of organic-inorganic hybrids having talc-like structure (TLH) through one single step. In this case, the organic chains are covalently linked to the silicon atoms of the tetrahedral sheets and are pending in the interlayer space and at the surface. TLH bearing propyl amino groups was shown to be an interesting material in the domains of depollution or drug delivery, where the intercalation of organic molecules such as dyes, drugs, and proteins was reported in literature [2]. Yet, achieving TLH having specific properties was previously shown to be highly influenced by the experimental conditions (solvent type and quantity, pH, reaction time, etc) of the synthesis procedure [3]. In the current study, the optimisation of the sol-gel process to obtain TLH bearing amino propyl groups has been investigated through testing several synthesis parameters. The structural and surface properties of the produced structures were characterized using a large scope of characterisation techniques (XRD, XRF, NMR, etc). In this work, a special attention was given towards the silica environment in TLH through the employment of ^{29}Si solid-state NMR to identify the different Si sites present (T^1, T^2, and T^3 shown in Figure 1) and thus determine their polycondensation degree. The latter was shown to be highly dependent on the solvent type and quantity but it was not very affected by the reaction time or by increasing the pH. These results open the possibility to synthetize hybrids with a tunable polycondensation degree using green solvents, low amounts of solvent, and less time.

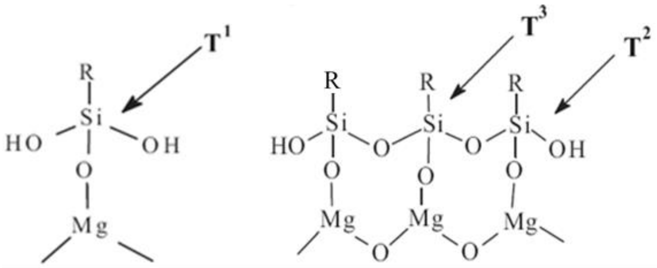

Figure 1. The different silica sites that can be present in the structure of TLH

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2D Inorganic Nanosheets and Nanohybrids for Energy Storage Technologies

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Highly anisotropic 2D nanosheets of layered inorganic solids (metal oxides, layered double hydroxides, metal chalcogenides, metal carbides, metal nitrides, metal phosphides, and carbon nitrides) have evoked great deal of research activity because of their outstanding performances as energy functional materials [1-5]. A great diversity in the chemical compositions, crystal structures, and defect structures of inorganic nanosheets provides this class of materials with a wide spectrum of physical properties and functionalities. The inorganic nanosheets can be used as powerful building blocks for exploring efficient energy-functional nanohybrids. Since the crystal defect and interfacial interaction have profound influence on the electrochemical activity of hybrid materials, the energy functionalities of 2D inorganic nanosheet-based hybrid materials can be greatly enhanced by defect- and interface-engineering. In this talk, several classes of 2D inorganic nanosheets and their nanohybrids applicable for renewable energy storage technology will be presented together with the discussion about the relationship between chemical bonding nature and functionalities. The crucial role of interface/defect engineering in optimizing the energy performances of 2D nanosheet-based materials will be highlighted.

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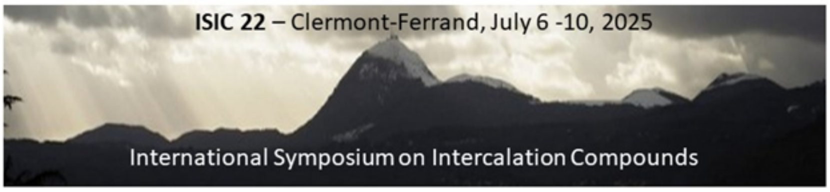

Advances in antioxidant Intercalated Layered Double Hydroxides for Polyolefins

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Hindered phenolic antioxidants have gained widespread recognition and application in enhancing the heat resistance and oxidative aging performance of polypropylene (PP) composites. However, the use of low molecular weight antioxidants poses certain challenges. These antioxidants have a greater tendency to volatilize, migrate, and be extracted from PP or PP-based products. Such behavior directly diminishes the anti-thermal oxidative aging efficacy of PP and its composites, and additionally presents a risk of contaminating food or drugs when used in packaging[1]. Layered double hydroxides (LDHs) are highly desirable as antioxidant protection materials due to their adjustable compositions (M^{2+} and M^{3+}) within the host sheet, replaceable interlayer anions (A^{n-}) in the interlayer region, and adaptable charge density (M^{2+}/M^{3+} ratio). Consequently, it is plausible to inhibit the migration of antioxidants utilizing host-guest interactions and supramolecular forces by intercalating low molecular weight hindered phenolic antioxidants into the interlayer gaps of LDHs. In our works, a series of antioxidant intercalated LDHs with excellent antioxidative and anti-migration performance were developed based on the adjustable multivariate structure and interlayer functional guest intercalation assembly characteristics of LDHs[2]. Particularly, breakthroughs in the one step synthesis of ultrathin antioxidant intercalated LDHs (L-LDHs), solvent blending, and other key technologies were achieved, realizing the precise preparation of a series of 1 ~ 10 layers ultrathin antioxidant intercalated LDHs and corresponding L-LDHs/PP composites. Besides, an efficient synthesis and organic-modification coupling strategy was developed to produce highly dispersed ultrathin antioxidant intercalated LDHs with low washing water consumption[3]. On this basis, a "fence" structure antioxidant intercalated LDHs at sheet edges and a chitosan encapsulation structure were created to further inhibit the migration behaviors of interlayer antioxidants. These advancements address industrial demands for durable, anti-migrating antioxidants, positioning PP for broader applications in harsh environments while ensuring safety and environmental compliance.

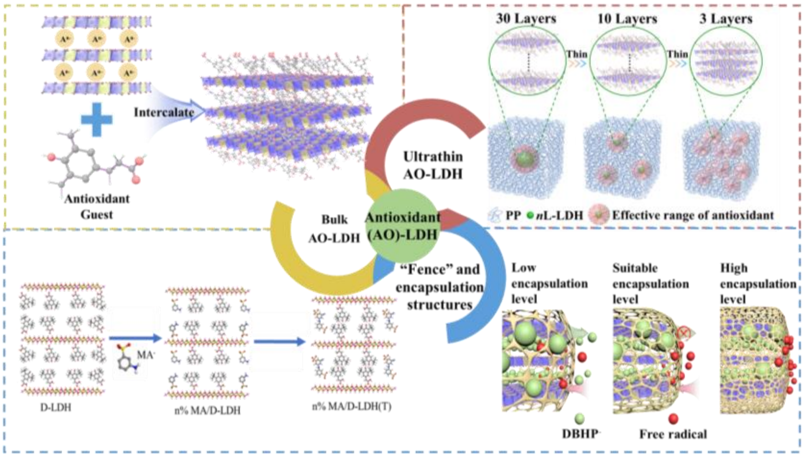

Figure 1. Advances in antioxidant Intercalated Layered Double Hydroxides.

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CFD Simulation of Multifluid Mixing in A Rotating Liquid Film Reactor for Magnesium Hydroxide Production

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Particle size distribution and morphology are very important in the application of nanomaterials, such as Layered Double Hydroxides (LDHs) and $Mg(OH)_2$. The rotary liquid film reactor (RLFR) has been invented by our group and used for the preparation of LDHs and $Mg(OH)_2$ with narrow particle size distribution in both laboratory and factories for more than 20 years[1].

In this paper, CFD was used to simulate fluid mixing and product formation during the synthesis of $Mg(OH)_2$ in a RLFR. The turbulence model was Standard k-ε model[2]. By simulating the mass fraction of generated $Mg(OH)_2$, the mixing efficiency of RLFR under different conditions can be obtained[3]. Especially by increasing the number of inlets, the uniformity of fluid distribution can be largely promoted, and the fluid mixing and mass fraction of $Mg(OH)_2$ can be obviously optimized. It was found that under the condition of four inlets, the inlet mass flow rate was 0.0003 $kg \cdot s^{-1}$ and the rotational speed was 5000 rpm, the production yield can be improved to 88.17%. According to the simulation results, a 4-inlet rotating liquid film reactor was manufactured for the preparation of nano-sized $Mg(OH)_2$. The results are in good agreement with the experiments. At 5000 rpm, the obtained $Mg(OH)_2$ products had regular crystal structure, uniform morphology and high dispersion, and the average particle size was 56.52 nm. This study provides a new approach and theoretical support for controllable preparation and performance optimization of nanomaterials using RLFR.

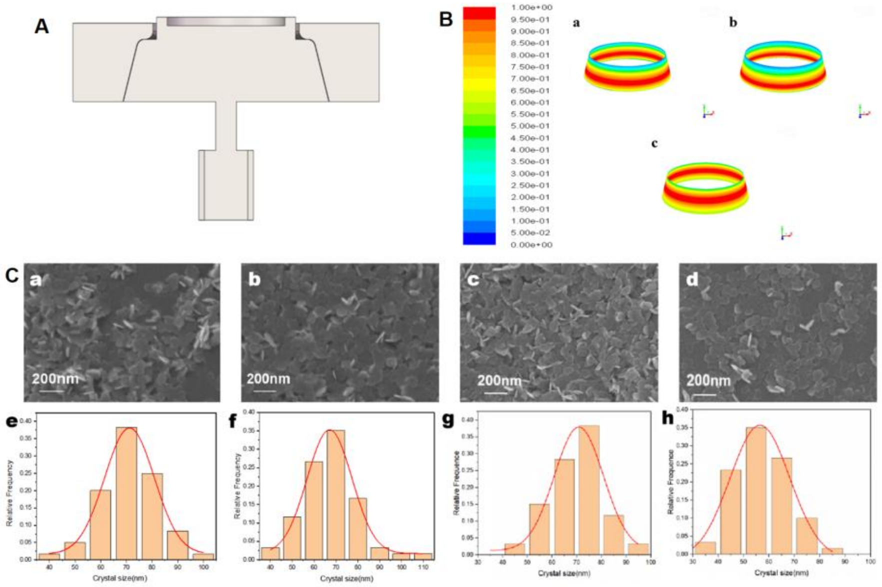

Fig 1. Geometry model of RLFR(A), mass fraction contours(B), SEM and primary particle size distribution(C) of $Mg(OH)_2$ with different inlets.

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Zirconium phosphates and sulfophosphonates intercalated by guanidine – synthesis, characterization and ionic conductivity

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Zirconium phosphates and phosphonates increasingly attract research interest due to their outstanding physical and chemical properties but also by their possible applications for example in catalysis, ion exchange, and proton conduction. Materials having high proton conductivity are important as they can be employed as a component of hydrogen fuel cells where they serve as membranes separating anode and cathode compartments. There are a number of strategies to influence the proton conductivity of layered substances: i) the guest itself can be modified using suitable organic substituents (carboxylic, sulfonic or amino groups), ii) suitable guests can be intercalated, interacting with the host groups and creating a network of hydrogen bonds capable of transferring protons, iii) a composite can be formed with a suitable polymer.

In this work, intercalates of guanidine into α- and γ-zirconium phosphates and α- zirconium phosphonates (4-sulfophenylphosphonate, 2-sulfoethylphosphonate) were prepared using guanidine chloride or carbonate by various methods (hydrothermal synthesis, host exfoliation). The products were characterized by powder X-ray diffraction, elemental analysis, IR spectroscopy and their ionic conductivity was measured.

Guanidine can be intercalated into zirconium sulfophenylphosphonates using both hydrochloride and carbonate at room temperature. For intercalation into zirconium phosphates, it is better to use guanidinium carbonate. All the intercalates contain about one guanidine molecule and one water molecule per formula unit and the presence of protonated guanidine in the interlayer space was confirmed by IR spectroscopy. The highest ionic conductivity was obtained for zirconium 2-sulfoethylphosphonate intercalate, the lowest one for γ-zirconium phosphate intercalate. The temperature dependence of conductivity was measured for both guanidine intercalated phosphonates.

The authors thank to the Czech Science Foundation (grant No. 23-06562S) for financial support.

Assembly of intercalated Layered Double Hydroxides with "fence" structure for enhancing anti-migration performance

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Polypropylene (PP) faces limitations in industrial applications due to auto-oxidative degradation caused by unstable α-hydrogens under environmental stressors [1]. Although antioxidants are commonly integrated to mitigate degradation, their migration compromises polymer integrity and poses environmental risks. Recent strategies utilizing layered double hydroxides (LDHs) to intercalate antioxidants via host-guest interactions have shown promise in reducing migration [2], yet long-term stability remains constrained by ion exchange and extraction. This study introduces a novel approach to enhance antioxidant confinement within LDHs by leveraging metanilic acid (MA), which undergoes in situ thermal polymerization to form a barrier-like "fence" structure at the interlayer edges. Through partial exchange of antioxidants with MA and controlled thermal treatment at 200°C, the resulting MA/D-LDHs(T) composite exhibited reinforced interlayer cohesion via hydrogen bonding and π–π stacking. This structural modification significantly suppressed antioxidant migration while maintaining high thermal and oxidative stability. Comprehensive characterization confirmed that the confined network effectively restricted guest mobility, thereby improving the anti-aging performance of PP composites. The optimized system demonstrated prolonged antioxidant retention and reduced environmental leaching, addressing critical challenges in conventional stabilization methods. By elucidating the mechanistic role of interlayer barrier formation, this work advances the design of durable, eco-friendly antioxidant systems for high-performance polymer applications, offering a scalable strategy to balance material longevity with sustainability.

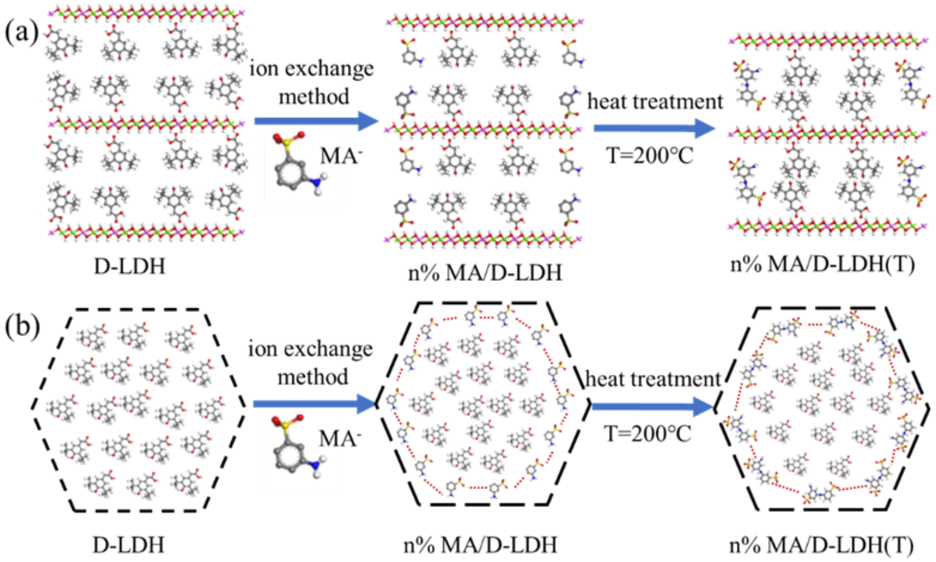

Figure 1. n% MA/D-LDH(T): (a) side view and (b) top view.

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The effect of the electrolyte concentration on the performances of Layered Double Hydroxides intercalated with Ferrocene anions

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Layered Double Hydroxides (LDHs) are a versatile class of 2D materials, which consist of layered di- and trivalent metal cation hydroxides with intercalated anions [1]. LDHs have been used very successfully for battery as well as supercapacitor energy storage application [2]. With our new approach, introducing redox active anions in between the layers of LDHs [3,4], we successfully intercalated ferrocene anions into the structure of $Mg_2Al(OH)_6$. Namely, FcMono and Fc-Di (Fig 1. A and B) with respective theoretical capacities of 60 $mA.h.g^{-1}$ and 40 $mA.h.g^{-1}$.

Although in first electrochemical tests, full theoretical capacities $Mg_2Al(OH)_6$-FcMono and $Mg_2Al(OH)_6$-FcDi have been measured in 1M aqueous electrolyte, a poor cycling stability due to the rapid dissolution of the reduced ferrocene anions into the electrolyte was obtained. It was possible to hinder this dissolution via the use of highly concentrated ionic liquids. This, however, came with the price of reduced specific capacities [5].

Therefore, in this work, we tried to optimize the capacity and the cycling stability of the material. To achieve this, it is necessary to find a compromise in electrolyte concentration. To reach the best performances, the electrolyte needs to combine high conductivity and properties of highly concentrated or highly viscous electrolytes to avoid the dissolution of the redox active anions. To do so, we tested $Mg_2Al(OH)_6$-FcMono and $Mg_2Al(OH)_6$-FcDi based electrodes in aqueous electrolytes and water-in-salt electrolytes (WiSEs) at different concentrations. Again highest specific capacities of the LDH active materials have been found in 1m LiTFSI in H_2O. On the other hand beginning from 5m electrolyte, very stable cycling was achieved for $Mg_2Al(OH)_6$-FcDi based electrodes (Fig 1. C and D), which was not possible for $Mg_2Al(OH)_6$-FcMono. This study highlights the necessity to optimize the electrolyte to unravel the full potential of novel electrode materials.

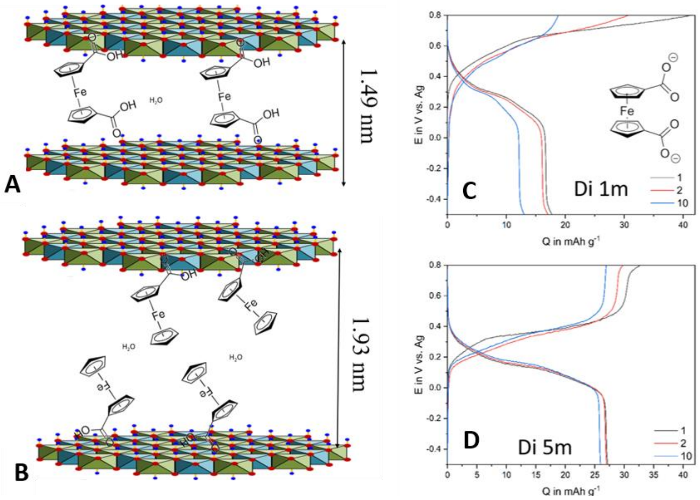

Figure 1: Schematic representation of the structure of A) MgAl-FcMono and B) MgAl-FcDi. Voltages profiles of charge/ discharge cycles 1, 2 and 10 for MgAl-FcDi based electrodes in C) 1m and D) 5m LiTFSI in H_2O at 1C.

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Ecologically Friendly 2D/2D Na^+-MXene/LDH for Cesium Adsorption in Salt Lakes: A Comprehensive Study on Adsorption Performance, Mechanisms, and Environmental Impact

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Cesium is a rare metal of paramount importance across various domains [1]. Despite abundant cesium resources in Qinghai-Tibet Plateau salt lakes, concentrations remain low, and existing adsorbents generally exhibit limited adsorption capacities [2]. Consequently, there is a pressing need for the development of an adsorbent capable of effectively separating and efficiently extracting cesium ions. This work utilizes the unique functional groups and negative charge characteristics of the two-dimensional (2D) MXene surface to promote the precipitation and crystallization of 2D layered double hydroxides (LDH), thereby enabling the in-situ growth of hydrotalcite on the MXene surface and synthesizing a 2D/2D stacked Na^+-MXene/LDH composite. The results indicated that Na^+-MXene/LDH exhibited enhanced specific surface area and interlayer spacing, introducing additional active sites that significantly improved Cs^+ adsorption capacity, with a maximum recorded uptake of 961.5 mg/g, surpassing previously reported MXene-based adsorbents. Adsorption tests conducted on brines from four hydrochemical types of salt lakes on the Qinghai-Tibet Plateau revealed that Na^+-MXene/LDH displayed the highest distribution coefficient (K_d^{Cs}) of 31.92×10^4 mL/g in Dong Taijnar Lake, demonstrating a strong affinity and selectivity for Cs^+. The mechanisms underlying the enhanced adsorption performance were elucidated. Additionally, ecological safety assessments, along with evaluations of microbial diversity and water quality in Qinghai Lake, confirmed that Na^+-MXene/LDH preserved microbial diversity and stabilized community structures, thereby underscoring its non-toxic and environmentally friendly characteristics. This research provides a promising adsorbent for cesium extraction from brine, with potential applications in water purification and ecological restoration.

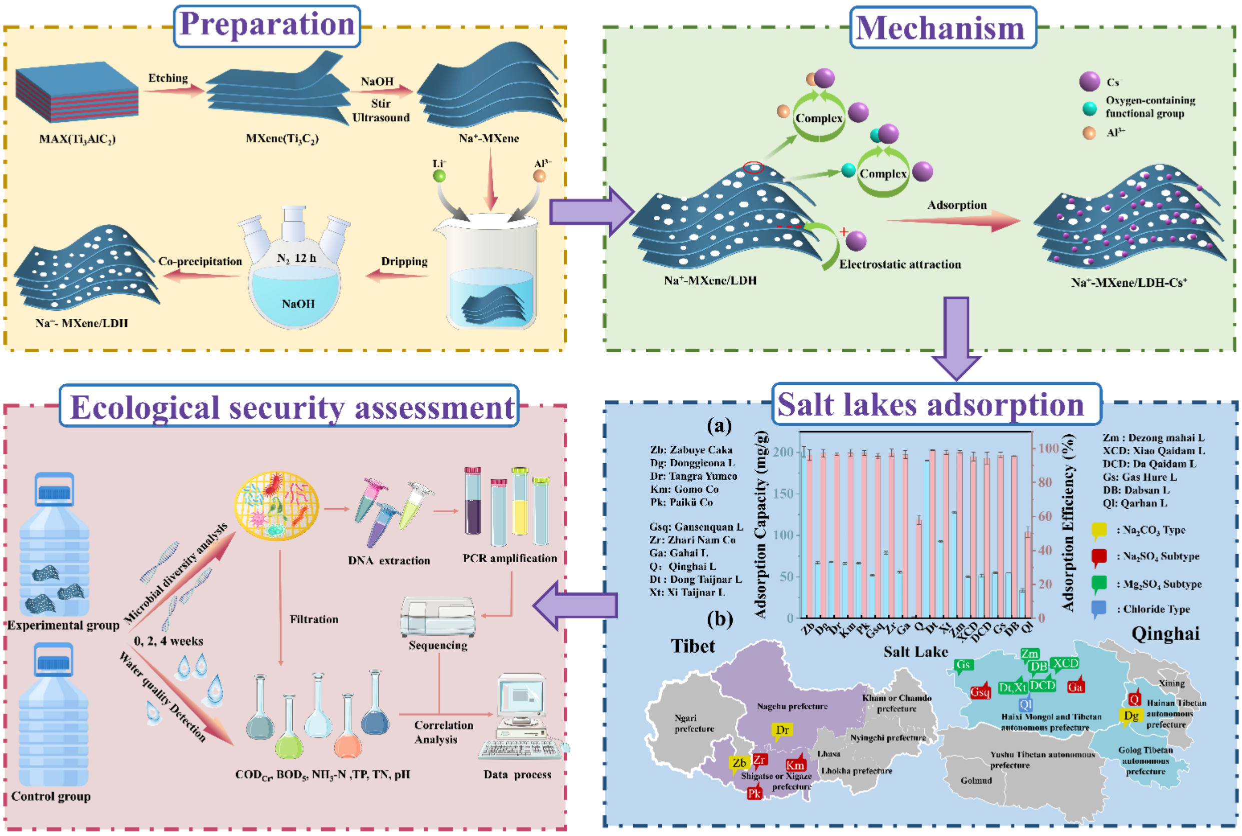

Fig 1. Graphical Abstract

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Enhanced CO_2 Hydrogenation Performance of Fe/Co-Based Nano Hydrotalcites for carbon neutral Fuels synthesis: A Study on Ultrasound-Assisted Synthesis and Catalytic Efficiency

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This study provides an exploration of the catalytic activity of novel Fe/Co/Cu-based nano hydrotalcite catalysts, synthesized through ultrasonic-assisted co-precipitation, in the context of Fischer-Tropsch mediated CO_2 hydrogenation (FTS-CO2) for the carbon neutral fuels synthesis.
The urgent need for carbon-neutral synthetic fuels has driven research into CO_2 hydrogenation via Fischer-Tropsch (FT) synthesis, where catalyst selection plays a crucial role in determining both conversion efficiency and environmental sustainability.
The distinctive physicochemical properties of these catalysts [1], which were extensively characterized by different techniques using XRPD, ICP-OES, SEM, TEM, FT-IR, BET, TPR, and TG, are responsible for their potential for CO_2 conversion with varied product distribution. The catalysts studied had the following molar fractions: Mg0.65Fe0.3Cu0.05 (Fe30), Mg0.55Fe0.4Cu0.05 (Fe40), Mg0.32Co0.33Fe0.3Cu0.05 (Co33), Mg0.24Co0.41Fe0.3Cu0.05 (Co41). The samples containing Co (Co33 and Co41) display greater catalytic activity and selectivity for heavier hydrocarbons (C7+) at all temperatures evaluated, ranging from 250 to 350°C. The differences in product distribution can be attributed to the unique physicochemical properties imparted by the ultrasonic co-precipitation method used in the catalyst's synthesis. At temperatures beneath 300 °C, the Fe30 catalyst exhibited about 10% higher CO_2 conversion compared to the Fe40 sample. The production of lighter hydrocarbons was predominant in both samples. At 300°C the four-catalysts tested demonstrated a reasonable trade-off between conversion rates, and synthesis of longer chain hydrocarbons. The outcomes from this observation provide a basis for further exploration into optimizing these catalysts for numerous CO_2 hydrogenation conditions.

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Enhanced Anti-Migration of Organic Antioxidants via Chitosan-Encapsulated Ultrathin Intercalated Layered Double Hydroxides Fabricated by a Nucleation-Encapsulation Coupling Strategy

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Antioxidants play a crucial role in inhibiting polypropylene (PP) oxidative damage and extending polymer lifetime.[1] However, the high migration rate and limited antioxidant efficiency significantly reduced their protective effects, and often forcing to overdose their quantity, which can then become a critical issue for the environment.[2] Herein, a more sustainable solution consists in using a new ultrathin antioxidant intercalated layered double hydroxides (LDHs) with chitosan (CS) encapsulation structure to block the migration of antioxidants by tuning the molecular CS weight to fully encapsulate each individual LDH unit. The optimized encapsulation level is identified to inhibit the migration of interlayer antioxidants without hindering the interlayer diffusion of radicals, thereby providing more sustainable protection for PP. An optimized composite 200kCS-3L-LDH/PP with the low molecular weight phenolic antioxidant (3,5-Di-tert-butyl-4-hydroxyphenylpropionic acid, abbreviated as DBHP) and encapsulated by CS of MW = 200k at an encapsulation level of 11.6wt%, which demonstrates a migration ratio as low as 8.17% after 204 h in absolute ethanol at 60 °C and overlong thermal aging resistance time (1920 min) under air atmosphere, thus far surpassing the conventional and most resistant product currently on the market 1010/PP (46.0% and 640 min, respectively). Such Russian doll composite structure offers a promising way to enhance PP with excellent anti-migration and antioxidative performance, and also provides a valuable strategy for the design and the controlled release if desired of interlayer ions in LDHs.

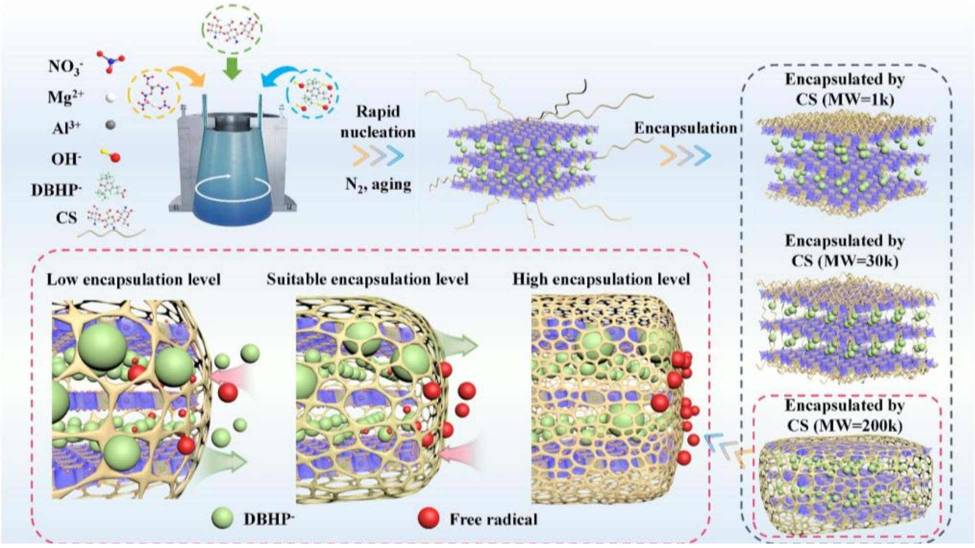

Figure 1. Inhibitory effects of encapsulation structures formed at different levels on the interlayer migration of DBHP.

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Topochemical silanization of the Aurivillius phase $Bi_2SrTa_2O_9$ and post-synthesis complexation of the interlamellar spacing

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The development of multifunctional layered hybrid materials extends across various research domains. Among these, layered perovskites (Aurivillius (AV), Dion-Jacobson (DJ), Ruddlesden-Popper (RP) type) are particularly promising, as their functionalization with organic compounds is well established. Our team previously demonstrated the possibility of grafting amines, alcohols[1,2] or even phosphonic acids[3] onto the AV phase $Bi_2SrTa_2O_9$, which exhibits ferroelectric and luminescent properties. Organosilanes are key components in hybrid material development due to their ability to form stable covalent bonds with inorganic surfaces, while introducing versatile functional groups capable of interacting with transition metals or other molecules of interest. Although organosilanes have been successfully grafted onto various layered materials (LDH, clays for instance), but their use remains uncommon for layered perovskites.

This poster presentation will demonstrate the grafting of three distinct organosilanes (3-(aminopropyl)triethoxysilane (APTES), N-[3-(trimethoxysilyl)propyl]ethylenediamine (TPED), and triethoxyoctylsilane (OTES)) onto the AV phase $Bi_2SrTa_2O_9$ using a multi-step microwave assisted approach. The grafting mechanisms within the perovskite layer are analysed using ^{13}C CP-MAS NMR and ^{29}Si MAS NMR, powder X-ray diffraction, and infrared spectroscopy. Furthermore, the ability of aminosilanes (APTES and TPED) to complex transition metals as copper or rare earth elements in confined spaces is explored, expanding the material's potential functionalities. To confirm this complexation, various spectroscopic techniques, including Electron Paramagnetic Resonance (EPR), UV/Vis absorption and photoluminescence spectroscopy, are employed.

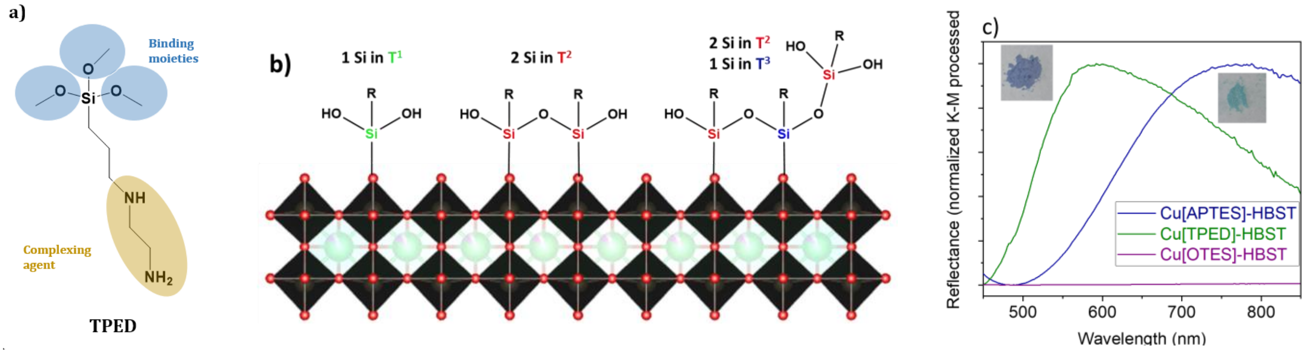

Figure: a) Molecular structure of TPED, b) Visual representation of the proposed grafting mode mechanism onto the perovskite layer, as deduced from ^{29}Si NMR analysis and c) UV/Vis reflectance spectra (Kulbeka-Munk processed absorbance) of the obtained product after reaction with copper

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Preparation of inorganic nanosheets and their application as high barrier packaging films

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Abstract

The key challenge in the circular economy relating to packaging materials is the removing of metallised film which is currently the industry standard approach with fulfilling barrier performance. Our team is particularly focused on the functionalization of inorganic nanosheets and their applications in recyclable packaging materials. We have developed a one-step method to efficiently prepare single-layer nanosheets using layered materials such as bimetallic hydroxides (LDHs), and reduced the preparation time from dozens of hours to 10 minutes. We also reported the synthesis of high aspect ratio 2D non-toxic layered double hydroxide (LDH) nanosheet dispersions using a non-toxic exfoliation method in aqueous amino acid solution. Then we discovered that aged layered double hydroxide nanosheet–polyvinyl alcohol dispersions can enhance gas barrier coating performance. High O_2 and water vapour barrier coating films were prepared using the dispersions above through a bar coating process, which is an existing commercial coating technique and easy for upscale production. The oxygen barrier performance of coated films has been improved by 40 times compared to commercial crisp packaging. The oxygen transmission rate can be reduced to less than 0.005 cc/m^2/day, and the water vapor transmission rate can be reduced to less than 0.04 g/m^2/day. Most importantly, these coated films are also transparent and mechanically robust, after mechanically flexed for 200 times according to international standards, its barrier performance remained basically unchanged, demonstrating its superior mechanical flexibility.

Keywords: High barrier packaging films; Composite materials; Nanosheets; Coating; Environmental protection

Sonochemical and mechanochemical as green routes for the preparation of layered double hydroxides

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Layered double hydroxides, (L DH) with general formula $[M(II)_{1-x}M(III)_x(OH)_2](A^{-n})_{x/n} \cdot mH_2O$, were M(II) is a divalent cation (i.e. Zn, Mg, Cu, Co), M(III) a trivalent cation (i.e. Al, Ga, Fe) and A^{n-} the anions that balance the positive charges of the lamellae, have attracted great interest thanks to the great variability of the intra- and interlayer composition. Catalytically active metal ions can be incorporated into the layer or immobilised on the surface through defect site engineering These materials can be used as catalysts or catalyst precursors to promote water splitting [1], Fischer-Tropsch reaction [2], biomass conversion [3], among others. Conversely, biomaterials can be obtained if the metal ions with therapeutic properties, such as anti-microbial and/or osteoconductive properties [4], are used as a component of the structure. Therapeutic efficacy can be enhanced by intercalation of bioactive species in the interlayer region. More recently, a new application of LDH has been envisaged as an additive to conventional cement pastes to improve durability. All of these applications at an industrial level can be actually realized through the implementation of green and scalable synthesis methods. Therefore, the possibility of producing LDH and modulating their layer composition and particle size using sustainable synthesis methods (especially in terms of production time and costs) is a task to be pursued. In this study, ultrasound-assisted and mechanochemical synthesis methods, considered green and efficient were employed for LDH preparation. The results were compared with those obtained using conventional co-precipitation at high supersaturation. LDH containing M(II) as Mg, Cu, Zn, Ni, Co and M(III) as Al, Ga, Fe have been prepared by the different methods and compared in terms of composition, phase purity, particle dimensions.

Furthermore, the impact on the reactivity of LDH prepared by different methods has been studied for NiFe LDH evaluating their catalytic performance as electrocatalysts for the oxygen evolution reaction (OER). These materials have been investigated for OER in alkaline media with various electrochemical measurements using in a single compartment three electrode cell.

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Construction of inorganic confining structures in layered double hydroxide interlayers for enhancing anti-migration performance

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Polypropylene (PP), a widely used industrial plastic, undergoes accelerated oxidative degradation due to unstable α-H bonds that generate free radicals (R• and ROOH) under thermal and UV exposure, leading to mechanical failure and surface deterioration [1]. While antioxidants mitigate degradation by scavenging radicals, their migration within the polymer matrix limits long-term efficacy and raises environmental concerns. Layered double hydroxides (LDHs) have emerged as promising carriers to immobilize antioxidants, leveraging their positively charged layers to stabilize negatively charged additives and reduce leaching [2]. However, existing LDH-antioxidant systems, such as co-precipitated DBHP$^-$intercalated LDHs, inadequately address migration resistance. This study introduces a novel anti-migration antioxidant with interlayer inorganic confining structure (C/D-LDH) engineered via partial ion exchange of D-LDH (prepared by nucleation/crystallization isolation) with Na_2CO_3. This strategy utilizes the narrow interlayer spacing originated from CO_3^{2-} in LDH to inhibit the outward migration of interlayer antioxidants. This unique architecture enhances interlayer confinement while preserving radical-trapping functionality. A series of n% C/D-LDH composites (n = 0, 4, 6, 8, 10, 12) were systematically evaluated for crystal structure, chemical bonding, and thermal behavior. Results revealed that optimized C/D-LDH incorporation significantly improved PP's thermal stability, delayed oxidation onset, and reduced antioxidant migration. Comparative analysis of PP composites containing C/D-LDH, DBHP/PP, and commercial Irganox 1010/PP demonstrated C/D-LDH's superior migration resistance. This work establishes a scalable strategy to balance antioxidant efficacy with migration suppression, advancing the design of durable, environmentally benign polymer composites for high-stress applications.

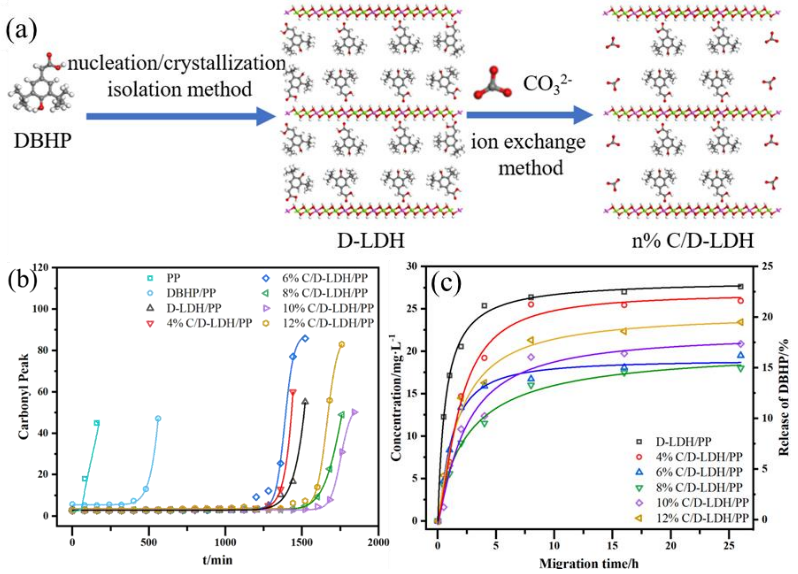

Figure 1. (a) Synthesis process diagram of n% C/D-LDH; (b) anti-thermal aging and (c) anti-migration performance.

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Synthesis and Characterization of Calcium Hydroxyapatite Composites Enhanced with Isoeugenol for Antibacterial Activity

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Calcium hydroxyapatite (CHA; $Ca_{10}(PO_4)_6(OH)_2$) is a widely recognized biomaterial known for its exceptional biocompatibility and bioactivity, making it highly suitable for various biomedical applications, especially in bone tissue engineering and dentistry [1,2]. Moreover, isoeugenol (ISOEUG), a naturally occurring phenolic compound and the isomer of eugenol, is known to demonstrate anti-inflammatory and anti-bacterial properties [3]. Therefore, this study focused on synthesizing and evaluating novel CHA composites with ISOEUG to examine their antibacterial properties. Composites were synthesized using the precipitation method. Techniques utilized to characterize the composites include X-ray diffraction (XRD), Fourier-transform infrared (FTIR) spectroscopy, thermogravimetric analysis (TGA), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Brunauer-Emmet-Teller (BET) surface area analysis, and liquid chromatography. The antibacterial efficacy of the samples was assessed against Gram-positive *Staphylococcus aureus* (*S. aureus*) and Gram-negative *Pseudomonas aeruginosa* (*P. aeruginosa*), and *Escherichia coli (E. coli)* using the inhibition zone method, particle size, zeta potential, and spot test. All samples demonstrated the typical XRD patterns of CHA (standard CHA PDF file No. 00-009-0432, shown as a vertical line in **Fig. 1** for comparison). FTIR spectra of pure ISOEUG and CHA/ISOEUG with different concentrations are displayed in the 4000-400 cm-1 region and presented in **Fig. 2**. The CHA/ISOEUG composites exhibited excellent antibacterial activity. These results highlight the effect of CHA with antimicrobial agents like ISOEUG, showcasing the potential of CHA composites as implant materials with antibacterial properties suitable for orthopedic and dental applications.

Keywords: Calcium hydroxyapatite, Composites, Isoeugenol, Antibacterial activity

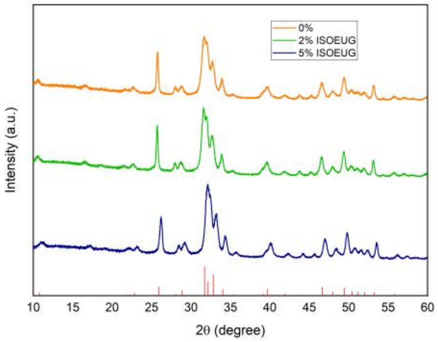

Figure 1: XRD patterns of CHA (ISOEUG 0%), and CHA/ISOEUG composites with 2% of ISOEUG; 5% of ISOEUG. Vertical lines represent the standard XRD pattern of CHA [PDF: 00-009-0432].

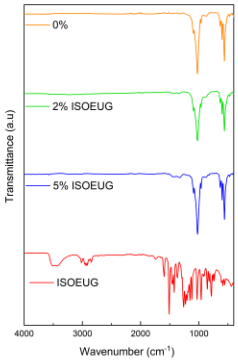

Figure 2. FTIR spectra of CHA (ISOEUG 0%), and CHA/ISOEUG composites 2% of ISOEUG, 5% of ISOEUG 5% and pure ISOEUG.

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Coordination Stabilization of Fe by Porphyrin-intercalated NiFe-LDH under Industrial-level Alkaline Conditions for Long-term Electrocatalytic Water Oxidation

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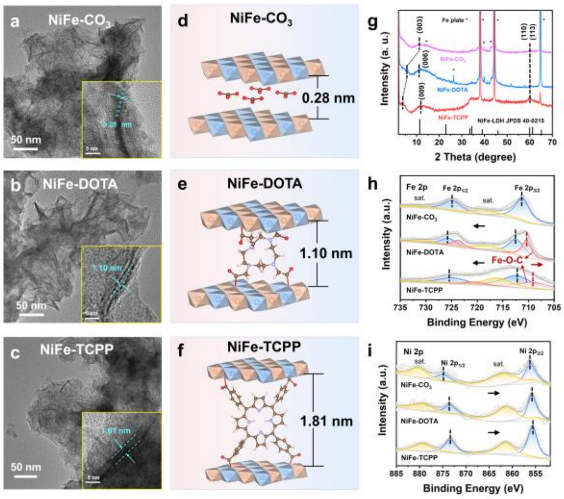
NiFe layered double hydroxide (NiFe-LDH) has long been regarded as one of the most promising alkaline OER catalysts due to its low cost and high activity. However, the industrial highly alkaline electrolyte exacerbates the Fe dissolution of NiFe-LDH, leading to the dramatic degradation of stability and activity. Therefore, stabilizing Fe species in NiFe-LDH is a critical challenge for industrial practical applications. To address this, The NiFe-LDH intercalated Tetrakis(4-carboxyphenyl)porphyrin (TCPP) (NiFe-TCPP) are fabricated for electrocatalytic water oxidation under industrial alkaline conditions. In 10 M KOH, the NiFe-TCPP exhibits ultralong stability for 1000 hours at the industrial current density of 500 mA cm^{-2} with a slight decay rate of 0.0093 mV h^{-1} and an ultralow overpotential of 290.2 mV at 1000 mA cm^{-2}. Moreover, the NiFe-TCPP-based anion exchange membrane water electrolyzer (AEMWE) displays excellent stability at 500 mA cm^{-2} and an operating cost of US \$1.44 kg$_{H2}^{-1}$ which lowers than the goal set by the US Department of Energy (<US \$2 kg$_{H2}^{-1}$). The theoretical and experimental studies reveal that the strong coordination not only drastically mitigates Fe dissolution by increasing the dissolution energy barriers and improving the self-healing ability, thus enhancing the stability, but also optimizes the d-band centers and decreases the OER energy barriers, thereby increasing the catalytic activity.



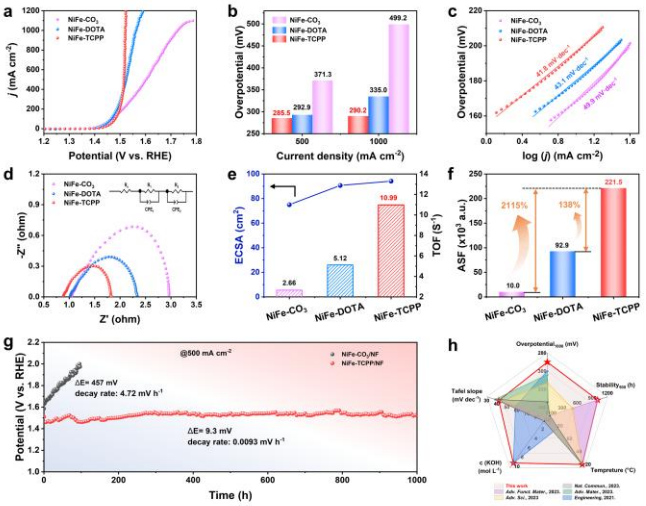


Figure 1. Structure characterization of NiFe-CO$_3$, NiFe-DOTA and NiFe-TCPP (right).
Figure 2. OER performance of NiFe-CO$_3$, NiFe-DOTA and NiFe-TCPP in 10 M KOH (left).

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Intercalation of photosensitizers in Zn_2Al-layered double hydroxide for water remediation

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Layered double hydroxides (LDHs), also known as anionic clays, have the general chemical formula $[M^{II}_{1-x}M^{III}_{x}(OH)_2]^{x+}[(A^{n-})_{x/n}\ .\ yH_2O]^{x-}$. They consist of positively charged metal hydroxide sheets where cations are located at the center of octahedra formed by hydroxides. Solvated anions (A^{n-}) are intercalated between these sheets. The compositional tunability of LDHs, enabled by the flexible selection of cations and intercalated anions (organic or inorganic), makes them highly versatile for various applications, with particular interest in water remediation [1]. In this context, the use of 2D systems, such as films formed either by *in situ* method or by particle deposition, is attractive as the materials can be recycled and reused. According to the literature, certain organic anions (benzoate, isophthalate, trimesate, etc.) intercalated into Zn_2Al-LDH through direct synthesis have been used as supramolecular photosensitizers, exhibiting photocatalytic properties in the near-infrared region [2]. These could allow the formation of highly reactive singlet oxygen $^1O_2$, to initiate the degradation of organic pollutants by oxidation mechanisms [3].

In this work, we investigated the intercalation of various anions (benzoate, phthalate, isophthalate, terephthalate, trimesate, trimellitate and pyromellitate) into Zn_2Al-LDH in two systems: films and suspensions. The hybrid organic-inorganic LDHs were synthesized using direct coprecipitation, anion exchange, and reconstruction. The arrangement of anions in the interlayer space was investigated as a function of (1) the synthesis method and (2) the system (whether particles were immobilised on a substrate or not) considering that the dynamic of the interlayer space may be constrained in the case of films [4]. The intercalation of organic anions in LDH materials was characterized by vibrational spectroscopies (Raman, IR), scanning electron microscopy (SEM) and X-ray diffraction (XRD). First, the successful intercalation of organic molecules was confirmed. Then, we demonstrated that the synthesis method influenced the microscopic structure of the materials (***Figure 1***). Finally, the anion stability in the interlayer space was studied in carbonate and chloride solutions to evaluate their exchange properties. The photocatalytic properties of the materials will be assessed in future studies.

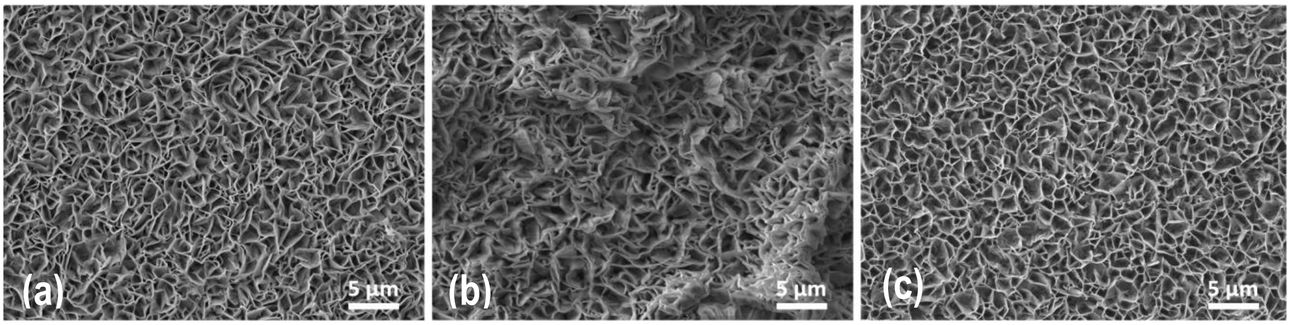

Figure 1: SEM images of (a) Zn_2Al-NO_3 LDH , (b) Zn_2Al-Benzoate LDH synthesized by exchange and (c) Zn_2Al-Benzoate LDH synthesized by reconstruction.

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single component, single layer flexile foam evaporator with the higher efficiency for water generation

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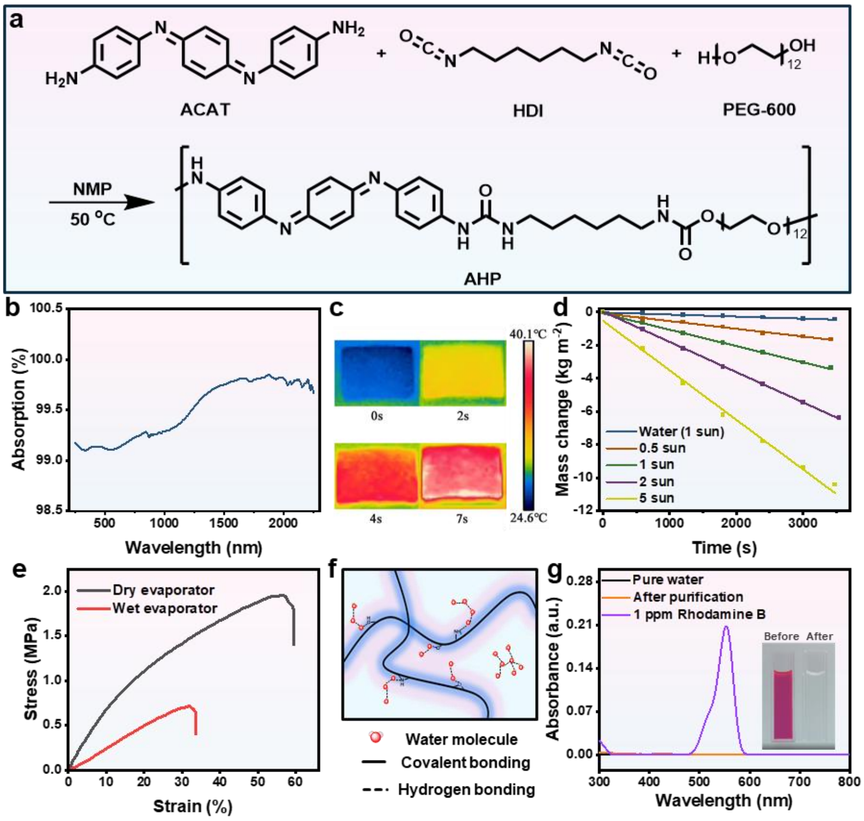
One of the greenest and promising ways to solve the problem of freshwater crisis is surface solar steam generation from seawater. A great number of photothermal materials with multi-component and multi-layered delicate yet complex structures often suffer from either low evaporation rate or high energy loss. Here, we present a single component foam evaporator with steam generation rate of up to 4.32 kg m^{-2} h^{-1} under 1 sun irradiation. The evaporator is constructed from an aniline oligomer as a single light-absorbing component, covalent linked with polyethylene glycol to form a monolithic polymer foam. Floating on the seawater, the foam has absorbance of 99.5% over the entire solar spectral range and low thermal conductivity (0.0077W $K^{-1}m^{-1}$) that effectively retains heat in the material and at the interface. After 3 months of continuous outdoor natural sunlight irradiation, the evaporator maintains a stable and durable evaporation rate. Moreover, the materials have good mechanical properties (7.48 MPa young's modulus and 57.38% elongation at break) and excellent chemical resistance in 10 common organic solvents and aqueous solutions of pH=1 to 14. This study provides a new system and strategy for desalination, steam power generation, treatment of polluted water and sewage, etc**.**



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Highly Luminescent Organic Phosphors Confined in LDH: A Rare-Earth Free Alternative for Solid-State Emission

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The development of optical devices often relies on coloured light-emitting diodes (LEDs), which are primarily composed of phosphors based on rare-earth elements. However, the extraction of these elements raises both environmental and geopolitical concerns.[1] To address this issue and design alternative rare-earth-free phosphors, our work focuses on the use of organic molecules exhibiting luminescent properties when excited under UV or blue light in dilute aqueous solutions. Despite their strong emission in solution, these fluorophores generally suffer from aggregation-caused quenching in the solid state (Fig.1 a).[2]

To overcome this limitation and obtain a solid-state phosphor, the luminescent molecules are co-intercalated within the structure of Layered Double Hydroxides (LDHs), alongside so-called spacer molecules.[3], [4] These spacers ensure a homogeneous dispersion of the fluorophores, mimicking the conditions of a dilute solution, and thus promoting intense luminescence in the resulting powders (Fig.1 b). By finely tuning the basal spacing of the LDH through the appropriate choice of spacers, optimal accommodation of the fluorophore is achieved, preventing its aggregation by maintaining sufficient intermolecular distances.

This design strategy, based on the selection of compatible spacers and fluorophores, leads to composite materials with high optical performance. Photoluminescence quantum yields reach up to 60%, and the powders demonstrate excellent thermal stability, making them promising candidates for future eco-friendly photonic applications.

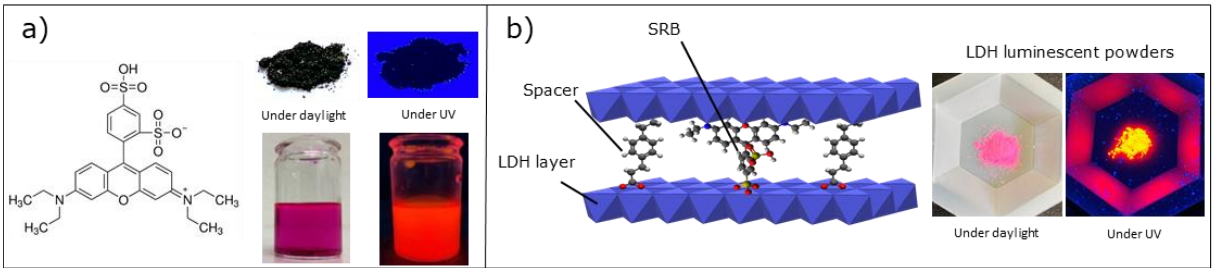

Fig.1 a) Structure of an example fluorophore (SRB) and its luminescence in solid state and in aqueous solution under daylight and UV light; b) Structure of the LDH-spacer-SRB and luminescence of the composite.

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Bimetallic Synergistic Effect of Co & Fe for the Highly Efficient Catalytic Decomposition of Ozone

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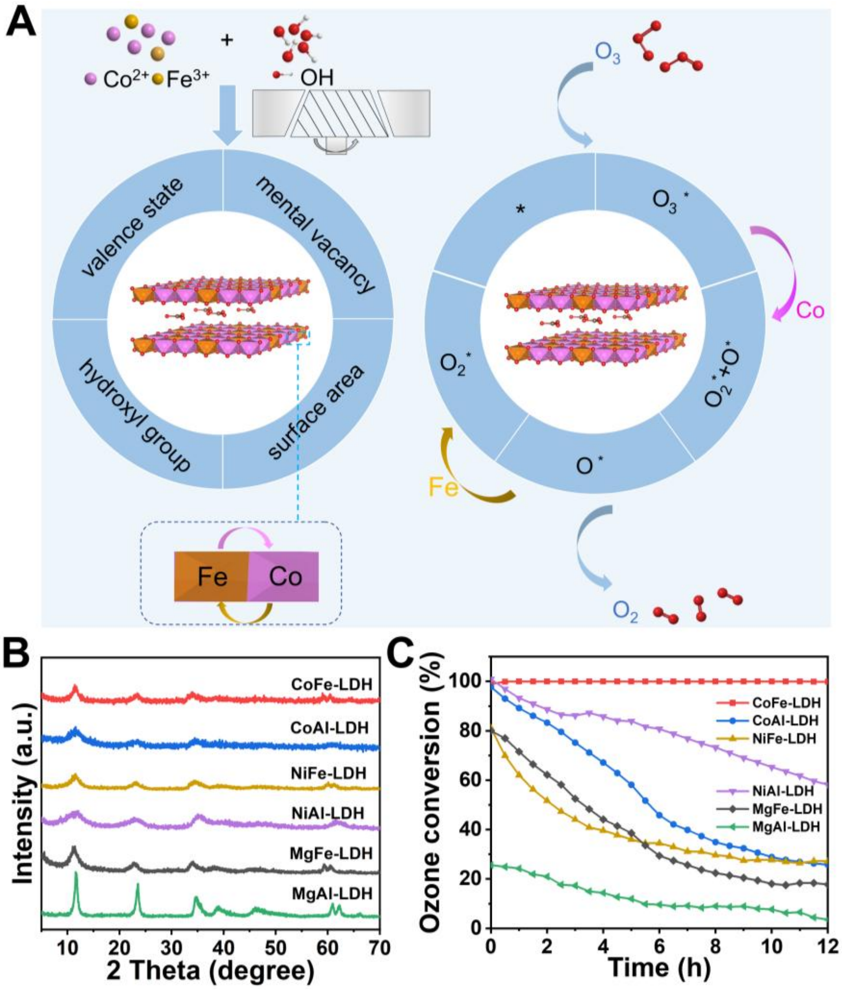
Ground-level ozone pollution is a major concern for human health, ecosystems, and material degradation. This paper presents a Co- and Fe-based bimetallic layered double hydroxide (CoFe-LDH) catalyst for ozone decomposition. The CoFe-LDH catalyst exhibited 100% ozone decomposition efficiency over 24 h at a reaction rate of 35.3 μmol g-1 min-1. The synergetic effects between Co and Fe regulated the valence state, increased the number of Co vacancies, and increased the specific surface area and density of the hydroxyl groups on the surface. Moreover, the two metals facilitated different dissociation steps and the desorption step became exothermic after ozone enrichment on the surface, rendering every step concurrently spontaneous, which has not been observed in previously reported ozone decomposition catalysts. This study demonstrates the potential of LDHs for ozone pollution control and offers new insights into the design of synergistic bimetallic catalysts.



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Tailoring LDH Morphologies for Advanced Catalytic and Antibacterial Applications

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Layered double hydroxides (LDHs) are incredibly versatile materials, finding applications in a wide array of fields such as catalysis, environmental remediation, and biomedical engineering [1]. Traditionally, when tailoring LDHs for specific applications, much attention has been given to the intercalated anion or the size of LDHs and how these factors influence their properties. However, morphology is equally important, having a significant impact on the direct properties of LDHs as well as of LDH-based composites. For instance, the sand-rose crystals exhibit enhanced catalytic activity and bactericidal efficiency due to their increased surface area and unique structural features [2]. Conversely, the plate-like crystals offer superior mechanical properties, making them ideal for use in composite materials [3].

This study delves into the modification of the urea method to synthesize LDHs through a streamlined one-step process, aiming to obtain distinct morphologies. The research focuses on several key parameters, including the urea/(Al + M(II)) molar ratio (R), reaction time, and metal salt concentrations. In particular, it was found that high R values and the use of nitrate salts promote the formation of sand-rose crystals, which are characterized by their intricate, flower-like structures. On the other hand, chloride salts lead to the development of plate-like crystals, which have a more uniform and flat appearance [4].

By understanding and manipulating the synthesis parameters, it is possible to tailor LDHs to meet the demands of various applications, thereby enhancing their overall performance and effectiveness, paving the way for advanced materials designed for targeted uses.

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Study of the high-pressure structure of fluoroperovskite : the lamellar post-perovskite

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Fluorine's high electronegativity promotes the unique structural and electronic properties of fluoride materials, such as strong anion-cation bonding and high lattice stability. These characteristics render fluoride materials highly sensitive to external parameters such as pressure, leading to rich polymorphism and varied phase behaviors. Increased interest in $NaM^{2+}F_3$ (M = Co, Fe, Mg, Mn, Ni, and Zn) orthorhombic perovskite materials has emerged because they exhibit lower transition pressures to the post-perovskite ($CaIrO_3$-type) phase compared to analogous oxides. Indeed, this transition requires extreme pressure and temperature conditions (125 GPa and 2500 K) [1]. Fluoride compounds lower the transition pressure tenfold allowing this phenomenon to be studied under laboratory conditions [2][3]. This phenomenon is particularly relevant to understanding seismic activity in the Earth's mantle, especially the D'' region, which is largely composed of $MgSiO_3$ undergoing a structural transition from the perovskite (Pv) 3D phase to the post-perovskite (pPv) 2D phase.

Several factors observed in oxides influence the Pv to pPv phase transition, most notable are the tolerance factor, octahedral tilt angles, and the pressure-transmitting medium. Shear strain, in particular, reduces the transition pressure. Martin et al. and Liu et al. studied the transition in $NaMgF_3$ using NaCl [4] and silicone oil [5], respectively. When the less hydrostatic medium (silicone oil) is used, the fluoroperovskite transitions near 19 GPa, whereas in the more hydrostatic medium (NaCl), the structural change occurs around 29 GPa.

Among the perovskites mentioned above, manganese-based $NaMnF_3$ has not yet exhibited a structural transition, despite two experimental studies [6-7]. In order to better understand its behaviour under pressure, a few microparticles obtained via the solvothermal route were studied in a diamond anvil cell with NaCl as the pressure medium, combined with X-ray diffraction. This study suggests that a transition may occur around 15 GPa, potentially leading to the pPv structure, although further investigation is required to confirm and fully understand this phenomenon. The next step is to scale up the process under optimized conditions using a multi-anvil press in order to precisely characterize the new structure.

Additionally, the influence of particle structuration on transition conditions is being investigated. $NaNiF_3$ nanoparticles were studied under the same conditions as $NaMnF_3$, using the same apparatus and parameters. While Yusa et al. observed a transition between 9,7 and 11 GPa with microparticles [2], no transition was detected up to 20 GPa with nanoparticles.

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Preparation of Well-defined Anatase Nanoparticles in a Nanoporous Polyimide Membrane for the Uniform Deposition of Platinum

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Titanium dioxide (TiO_2) is a well-known wide-band-gap semiconductor used as pigments and as catalysts for energy production and environmental purification.[1] The particle size affects the dispersion stability, light scattering, and surface area, so the size-controlled syntheses have been reported.[2] Co-catalysts have been reported to improve the photocatalytic activity of anatase particles, where the size and spatial distribution of the co-catalyst nanoparticle affect the photocatalytic activity.[3] In this study, a nanoporous polyimide membrane with the pore diameter of ca. 50 nm was utilized as the template to obtain anatase nanoparticles with the size of ca. 16 nm by the infiltration of tetraisopropoxy titanium(IV) into the pore and the subsequent heat treatment at 500 °C. Pt was deposited on the anatase nanoparticles for H_2 evolution from aqueous methanol. The optimum Pt loading for the H_2 evolution was 0.1 wt%, which is lower than the commonly reported value (1 wt%) of the Pt loading on anatase.[4]

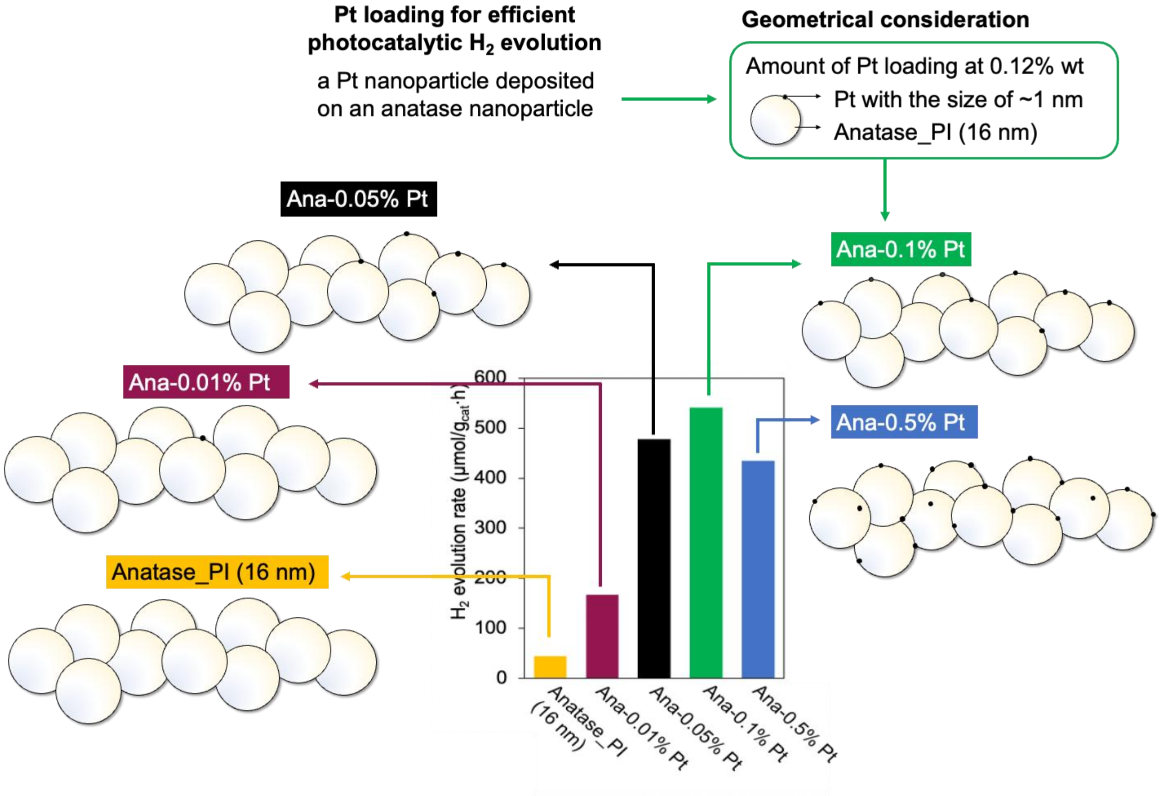

Figure 1 Schematic Illustration of the location of Pt on the anatase corresponding to the H_2 evolution rate

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Preparation and characterization of new layered zirconium aminophosphonates

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Layered zirconium organophosphonates represent an important group of inorganic-organic hybrid compounds due to their excellent stability and the possibility to modify the organic part of these compounds with functional groups. Zirconium phosphonates functionalized with acidic groups were extensively studied,[1] but much less attention has been paid to phosphonates bearing basic groups. The structure of zirconium 2-aminoethylphosphonate was solved and its intercalation behavior was described.[2,3] The preparation of other aminoalkylphosphonates was described, but no information about basal spacing was published.[4] In this work, zirconium 3-aminopropylphosphonates were prepared using various zirconium sources (oxychloride, acetylacetonate, propoxide) and reaction conditions (80 or 160°C, presence of acetic or phenylboronic acid).

If zirconium oxychloride is used as a zirconium source, only $Zr(O_3PC_3H_6NH_2)_2{\cdot}2HCl$ is obtained, regardless of the other acid used.

Compound $Zr(O_3PC_3H_6NHCOCH_3)_2$ with a basal spacing of 18.45 Å was prepared solvothermally from zirconium propoxide or acetylacetonate in the presence of acetic acid at 180 °C. Its IR spectrum shows bands characteristic for amides, which means that the amino group of the phosphonate reacted with acetic acid forming an amide during the synthesis of the sample. If the same reaction is done at 80°C, the product has a basal spacing of 19.5 Å and contains protonated amino groups and acetate anions. No formation of amide was observed by IR spectra.

If the phenylboronic acid, which is not able to react with amino group, was used, the compound $Zr(O_3PC_3H_6NH_2)_2{\cdot}2C_6H_5BO_2H_2$ with the basal spacing of 23.52 Å was prepared at both temperatures.

It was shown, that preparation of pure zirconium 3-aminopropylphosphonate from its hydrochloride form is difficult, but according to our preliminary experiments the samples containing acetate or phenylboronate anions could be used for an anion exchange.

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Design of new luminescent hybrid materials based on layered oxides

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The design of hybrid materials to achieve new functionalities constitutes a highly researched area.[1] These materials have proved to be very relevant, combining the strengths of the two realms, organic and inorganic, while compensating the drawbacks. Especially in the field of luminescent materials, organic compounds generally exhibit good luminescence quantum yields, and their structure can be easily and finely modulated to allow adjustment of their optical properties (excitation and emission wavelengths, or lifetimes of excited states). However, they are often relatively unstable, either chemically or thermally, and are prone to photo-bleaching.

In this respect, the combination of luminescent organic molecules with inorganic structures is particularly interesting, as it combines the advantages of organic systems (structural versatility, property tuning) with those of inorganic compounds (thermal stability, structural rigidity).[2] It may also bring improved properties to the hybrid material thus formed, such as better control of luminescence lifetime.

The present study involves two key steps: first, the insertion of simple alkylamine or alcohol chains as spacers in a pre-functionalisation process followed by the incorporation of large chromophores into the Aurivillius $Bi_2SrTa_2O_9$ and Dion-Jacobson $RbLaNb_2O_7$ phases via their protonated forms ($H_2Bi_{0.1}Sr_{0.85}Ta_2O_7$, HBST, and $HLaNb_2O_7$, respectively). The chosen chromophores are derived from 1,8-naphthalimide and (2)/(4)-bromo-1,8-naphthalimide, which exhibit Thermally Activated Delayed Fluorescence (TADF) properties,[3] and functionalised by different anchoring groups. Additionally, the Aurivillius $Bi_2SrTa_2O_9$ phase has been observed to exhibit persistent luminescence[4,5] under certain conditions, merely due to Bi^{3+}, although its origin remains unclear. Interestingly, even the insertion process itself appears to influence this luminescence. Thus, more research on this subject have been done.

I will describe the structural characterisation of the obtained hybrid compounds. Then I will discuss their photophysical properties, notably the emission wavelength, quantum yield, lifetime and the various parameters that could tune their photophysical properties (insertion rate, co-insertion, nature of the chromophore). Such approach has been described in the case of Layered Double Hydroxide-based hybrids,[6,7] but to the best of our knowledge has not been attempted for layered oxides, which exhibit peculiar features.

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First preparation of fluorinated diamane-type materials by ball-milling in a liquid phase

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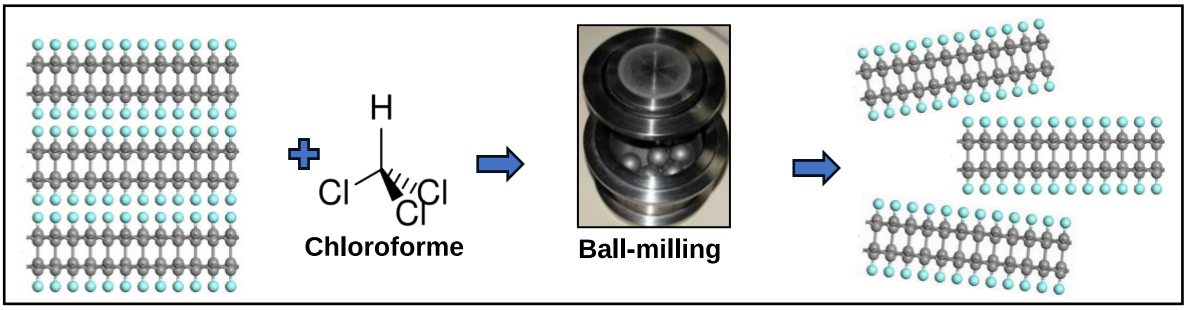
Diamonds are well known for being one of the hardest materials found in nature. Its metastability and its conversion into graphite are more prevalent at the nanometric scale, e.g. with single layered diamond then called *diamane* [1]. This emerging nanomaterial cannot be synthesized directly without abnormal pressure and/or temperature to stabilize its' sp^3 hybridized structure. Another way to stabilize both the structure and sp^3 hybridization of the carbon atoms is to introduce hetero elements onto its surface like H or F, resulting in fluorinated *F-diamanes* or hydrogenated H-*diamanes[2].* The *F-diamane* is a two-dimensional carbon-based fluorinated material whose physical properties rival that of the diamond [3]. Keeping its carbons hybridized to sp^3 as well as the very low thickness close to a 2-layered graphene.

Keeping in mind that *F-diamane* layer is the building unit of the 'stage-2' graphite fluoride with $(C_2F)_n$ structural type and composition $CF_{0.5}$[4], we propose to use a top-down synthesis of the *F-diamane*-type materials by exfoliation. Firstly, the fluorination conditions of graphite with molecular fluorine (F_2) are selected to prepare the $(C_2F)n$ phase [5]. The resulting material is then mechanically exfoliated by ball milling in chloroform. The shearing forces of the grinding provide enough energy to separate the layers of $(C_2F)_n$ which are then collected (dispersed) in the liquid. Complementary techniques evidence the preparation of stable *F-diamane* dispersion without damage due to the ball-milling. Moreover, the F-diamane-type layers exhibit lateral size of in the 1-5 μm range. Using either the dispersion or the layers after removal of the liquid, the properties of F-diamane-type materials can be investigated, e.g. photoluminescence, tribological, thermal, paramagnetic.

Image 1: Exfoliation of F-Diamane



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Application of layered and porous materials of biogenic origin in the removal of heavy metals and organic pollutants from water

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Environmental contamination caused by several pollutants has emerged as a profound global challenge with far-reaching implications for public health and ecological sustainability.[1] Heavy metals are exceptionally dangerous due to their persistence in nature, high potential for bioaccumulation, and toxicity even at trace levels, leading to neurotoxic effects, carcinogenesis, and severe developmental disorders in exposed populations. Organic compounds such as polychlorinated biphenyls (PCBs), endocrine inhibitors, glyphosate, and polycyclic aromatic hydrocarbons (PHAs) disrupt critical biochemical pathways, often causing chronic health issues. These pollutants intertwine to create complex contamination scenarios that traditional remediation strategies often fail to address effectively. In response, the development of new materials that are both sustainable and efficient in capturing and degrading these pollutants is more imperative than ever. Materials of biogenic origin are pivotal for sustainable innovation, as they convert waste by-products into eco-friendly, cost-effective solutions that curb pollution and bolster circular economic models. In light of these considerations, within the NODES Project (Northwest Digital And Sustainable), an innovation ecosystem funded by the Italian Ministry of Education, Universities and Research or MUR (PNRR, D.D. n.1054 of June 23, 2022), a series of synthetic layered clays (saponites) and porous silicas (MCM-41 and SBA-15), prepared from rice husk processing, were tested in the removal of various inorganic and organic pollutants from water media, including: **1)** heavy metal ions (Al, As, Cd Cr, Cu, Fe, Hg, Ni, Mn, Pb and Zn, at 0.1 mg/L), **2)** PAHs, PCBs and nitro-PHAs (9 ng/L, 0.101 µg/L); **3)** glyphosate (2 mg/L); **4)** endocrine disruptors (4-nonylphenol at 1 µg/L, bisphenol A at 5 µg/L). Contact tests were performed in mild conditions (T_{amb}, P_{amb}, under stirring), with a solid/liquid ratio of 5.71. Analogues materials obtained from traditional synthesis were also tested as reference solids. After 24 h, analyses were performed on the treated water samples using proper analytical techniques. Overall, all solids show promising results in removing target contaminants such as heavy metals (Fig. 1), PCBs, PHAs and nitro-PHAs. Current studies focus on the analysis of actual contaminated water samples provided by regional water companies.

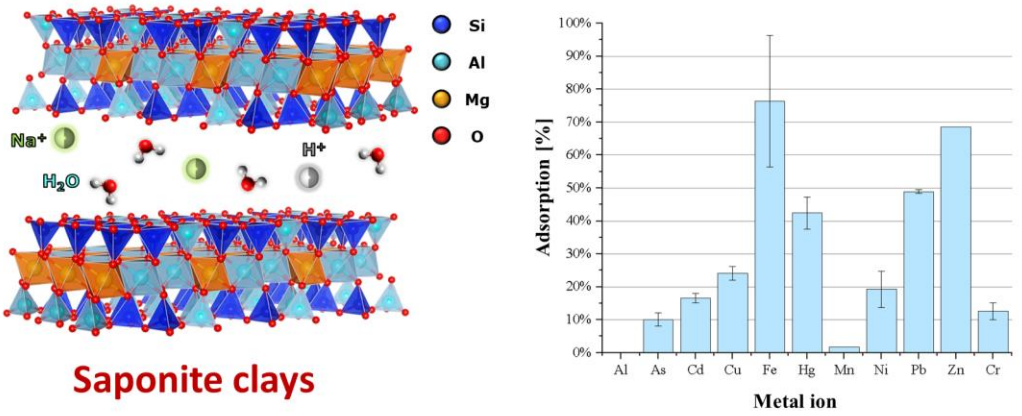

Figure 1. Selectivity test on the removal of different metal ions from water ($[C]_{Me}$ = 0.1 mg/L) using a synthetic saponite clay prepared in this study.

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Synthesis and Characterization of Calcium Hydroxyapatite Composites Enhanced with Isoeugenol for Antibacterial Activity

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Calcium hydroxyapatite (CHA; $Ca_{10}(PO_4)_6(OH)_2$) is a widely recognized biomaterial known for its exceptional biocompatibility and bioactivity, making it highly suitable for various biomedical applications, especially in bone tissue engineering and dentistry [1,2]. Moreover, isoeugenol (ISOEUG), a naturally occurring phenolic compound and the isomer of eugenol, is known to demonstrate anti-inflammatory and anti-bacterial properties [3]. Therefore, this study focused on synthesizing and evaluating novel CHA composites with ISOEUG to examine their antibacterial properties. Composites were synthesized using the precipitation method. Techniques utilized to characterize the composites include X-ray diffraction (XRD), Fourier-transform infrared (FTIR) spectroscopy, thermogravimetric analysis (TGA), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Brunauer-Emmet-Teller (BET) surface area analysis, and liquid chromatography. The antibacterial efficacy of the samples was assessed against Gram-positive *Staphylococcus aureus* (*S. aureus*) and Gram-negative *Pseudomonas aeruginosa* (*P. aeruginosa*), and *Escherichia coli (E. coli)* using the inhibition zone method, particle size, zeta potential, and spot test. All samples demonstrated the typical XRD patterns of CHA (standard CHA PDF file No. 00-009-0432, shown as a vertical line in **Fig. 1** for comparison). FTIR spectra of pure ISOEUG and CHA/ISOEUG with different concentrations are displayed in the 4000-400 cm-1 region and presented in **Fig. 2**. The CHA/ISOEUG composites exhibited excellent antibacterial activity. These results highlight the effect of CHA with antimicrobial agents like ISOEUG, showcasing the potential of CHA composites as implant materials with antibacterial properties suitable for orthopedic and dental applications.

Keywords: Calcium hydroxyapatite, Composites, Isoeugenol, Antibacterial activity

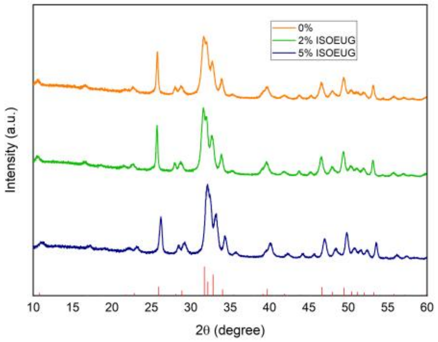

Figure 1: XRD patterns of CHA (ISOEUG 0%), and CHA/ISOEUG composites with 2% of ISOEUG; 5% of ISOEUG. Vertical lines represent the standard XRD pattern of CHA [PDF: 00-009-0432].

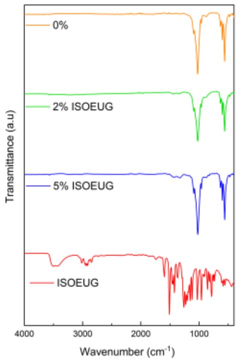

Figure 2. FTIR spectra of CHA (ISOEUG 0%), and CHA/ISOEUG composites 2% of ISOEUG, 5% of ISOEUG 5% and pure ISOEUG.

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Use of the Memory Effect of Hydrotalcites for the Preparation of Composite Anion Exchange Membranes for Electrolysis

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Hydrogen production through water electrolysis using polymeric membranes is a promising approach for sustainable and clean energy applications. Among the different electrolysis technologies, Anion Exchange Membrane Electrolyzers (AEMELs) have gained increasing attention as a cost-effective alternative to conventional alkaline electrolyzers and Proton Exchange Membrane Electrolyzers.[1] Anion Exchange Membranes (AEMs) operate in an alkaline environment, where the transport of hydroxide ions (OH^-) plays a crucial role in determining the efficiency and durability of the electrolysis process. However, traditional polymeric AEMs often suffer from stability issues due to the degradation of quaternary ammonium groups under alkaline conditions, leading to reduced performance over time. To overcome these limitations, layered double hydroxides (LDHs) have been investigated as promising inorganic fillers to enhance the mechanical strength, ion exchange capacity, and ionic conductivity of composite AEMs. LDHs are a class of two-dimensional (2D) anionic clays also known for their unique “memory effect,” wherein they can be thermally decomposed into layered double oxides and subsequently regenerated in aqueous solutions containing appropriate anions.[2] In this work, we investigate the synthesis and the characterization of MgAl, NiAl, and ZnAl-based LDHs, with a specific focus on their thermal behavior and rehydration properties through the memory effect and the potential of these materials as functional fillers in composite AEMs for electrolysis applications, particularly AEMELs. The experimental results confirm that MgAl-based LDHs exhibit the most effective structural regeneration after calcination at different temperatures, with superior ion exchange capacity (IEC), mechanical strength, and stability under alkaline conditions. The incorporation of MgAl-LDH fillers in the AEMs improves their mechanical and swelling properties while maintaining good ion conductivity. Overall, the use of LDH-based fillers obtained via the memory effect represents a promising strategy to enhance the mechanical robustness and ion transport properties of composite AEMs. Further studies on the long-term stability and conductivity optimization of LDH-filled membranes could significantly contribute to the advancement of high-performance and durable anion exchange membranes for applications in alkaline fuel cells and water electrolysis, supporting the transition to sustainable energy solutions.

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Highly Exposed Low-Valence Ni sites of NiO(111) for Efficient Electrocatalytic Biomass Upgrading

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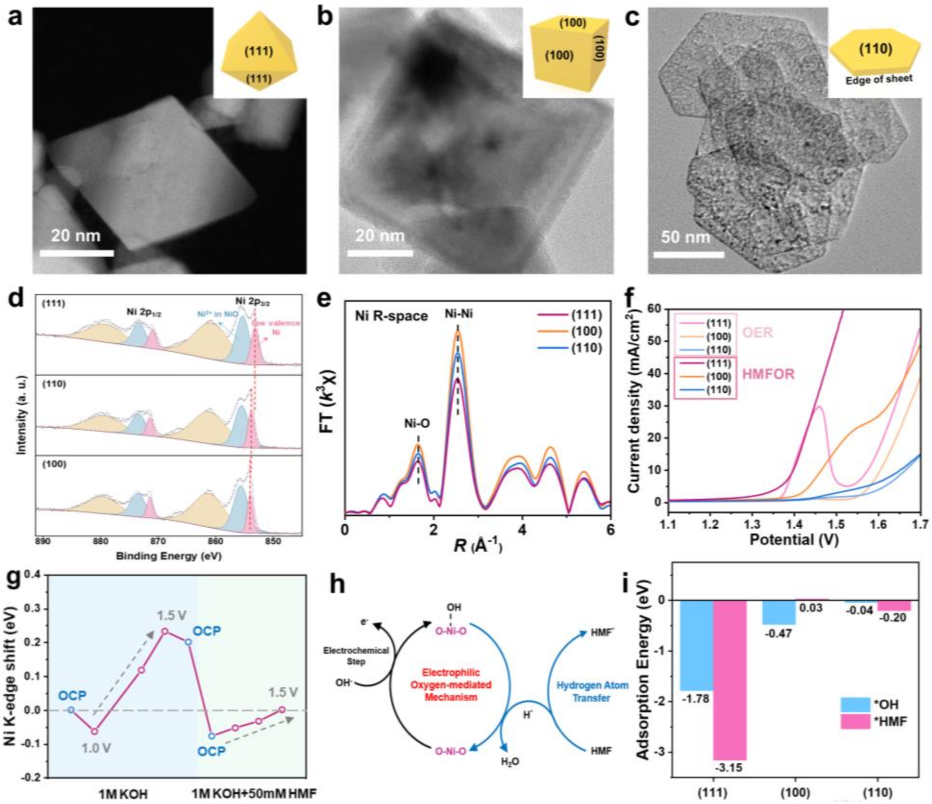
The catalytic activity of transition metal oxides (TMOs) is significantly influenced by the exposure of different crystal facets due to the distinct arrangements of surface atoms. However, the detailed structural change of TMOs with specific exposed facet and the corresponding structure-activity relationship remain ambiguous. In this work, we successfully fabricated the NiO catalysts with different facet exposure, including (111), (100) and (110). When applied for the structure-sensitive electrocatalytic 5-hydroxymethylfurfural oxidation reaction (HMFOR), the as-prepared NiO(111) exhibited a low onset potential of 1.23 V and achieved a current density of 10 mA cm^{-2} at 1.39 V. Moreover, it realized over 99% HMF conversion and approximately 99% selectivity of FDCA. Detailed in-situ experiments demonstrated that the electrooxidation of HMF on NiO requires the simultaneous fulfillment of hydroxyl adsorption and strong affinity for HMF. Further, characterizations and DFT calculations confirms that NiO(111) with numerous exposed and continuous low-valence Ni sites can realize both hydroxyl adsorption with lowest adsorption energy of -1.78 eV and sufficient affinity sites for HMF with d-π interactions. Additionally, the unique atomic arrangement of NiO(111) with the most pronounced charge transfer demonstrated superior charge transfer capability compared to (100) and (110). This work provides insights into the fine structure and surface evolution process of NiO with different exposed facets, and offers guidance for designing active Ni sites for efficient electrocatalytic biomass conversion.



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Simultaneous Mineralization of Cd(II), Pb(II) and As(V) Using MgAl-NO_3: Performance and Mechanism

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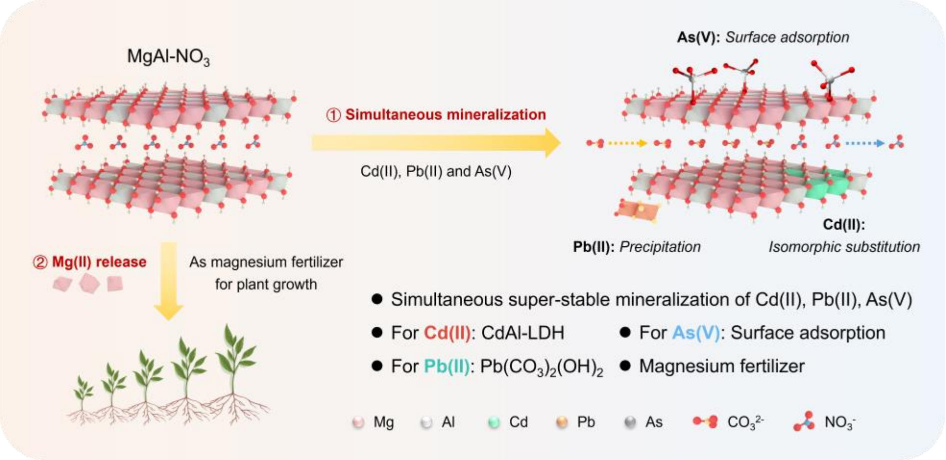
Water and soil contaminated by multiple heavy metal cations and anions such as Cd(II), Pb(II) and As(V) constitutes a serious environmental issue due to their toxicity, ubiquity and non-biodegradability. Herein, a MgAl-layered double hydroxide intercalated with nitrate (MgAl-NO_3) was successfully fabricated, which showed the maximum mineralization capacities (q_m) of 334.45, 1156.25 and 168.63 mg g^{-1} towards individual Cd(II), Pb(II) and As(V) in aqueous solution, respectively, outperforming most mineralizers reported so far. The mineralization data can be well fitted with the pseudo-second-order kinetic and Langmuir isotherm models. For the co-existence system of Cd(II), Pb(II) and As(V) in solution, the removal efficiency can reach 95% in 20 h by using MgAl-NO_3. Further application of MgAl-NO_3 for co-existing heavy metals polluted soil, 79.25%, 64.75% and 62.00% of available Cd, Pb and As in soil were mineralized in only two weeks, respectively. Accompanied by the mineralization of heavy metal cations and anions, the Mg(II) ions can be released from MgAl-NO_3 to promote azuki bean seedling growth as fertilizer. Detailed characterization indicated that the Cd(II) was anchored in the laminate of MgAl-NO_3 by isomorphic substitution, resulting in the formation of CdAl-LDHs; the Pb(II) was removed as $Pb_3(CO_3)_2(OH)_2$; surface adsorption dominated the mineralization process for As(V) removal. This work paves a new pathway for remediation of the co-existing heavy metal cations and anions in both water and soil.



Ultrathin NiV Layered Double Hydroxide for Methanol Electrooxidation: Understanding the Proton Detachment Kinetics and Methanol Dehydrogenation Oxidation

Z. H. Wu,[1] S. Bai,[1] T. Y. Shen,[1] G. H. Liu,[1] Z. H. Song,[1] Y. H. Hu,[1] X. L. Sun,[1]
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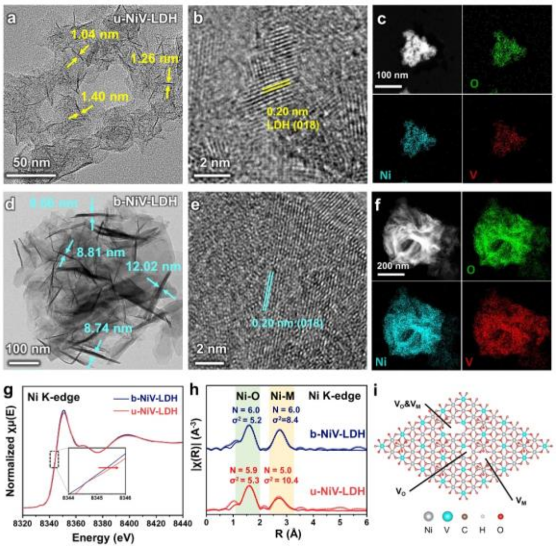
Electrochemical methanol oxidation reaction (MOR) is regarded as a promising pathway to obtain value-added chemicals and drive cathodic H_2 production, while the rational design of catalyst and in-depth understanding of the structure-activity relationship remains challenging. Herein, the ultrathin NiV-LDH (u-NiV-LDH) with abundant defects is successfully synthesized, and the defect-enriched structure is finely determined by XAFS *etc*. When applied for MOR, the as-prepared u-NiV-LDH presents a low potential of 1.41 V *vs.* RHE at 100 mA cm^{-2}, which is much lower than that of bulk NiV-LDH (1.75 V *vs.* RHE) at the same current density. The yield of H_2 and formate is 98.2% and 88.1% as its initial over 5 cycles and the ultrathin structure of u-NiV-LDH can be well maintained. Various *operando* experiments and theoretical calculations proves that the few-layer stacking structure makes u-NiV-LDH free from the interlayer hydrogen diffusion process and the hydrogen can be directly detached from LDH laminate. Moreover, the abundant surface defects upshift the d-band center of u-NiV-LDH and endow a higher local methanol concentration, resulting in an accelerated dehydrogenation kinetics on u-NiV-LDH. The synergy of the proton detachment from the laminate and the methanol dehydrogenation oxidation contributes to the excellent MOR performance of u-NiV-LDH.



(a-b) HRTEM and (c) elemental mapping of b-NiV-LDH; (d-e)HRTEM image and (f) elemental mapping of u-NiV-LDH; (g) XANES spectra of Ni K-edge; (h) magnitude of weighted FT of Ni K-edge EXFAS (point plots) and fitting curves (solid lines); (i) the schematic illustration of defect structure of u-NiV-LDH.

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Synthetic Application of Immobilized Chiral Secondary Amine Catalysts and Impregnated Palladium Nanoparticles

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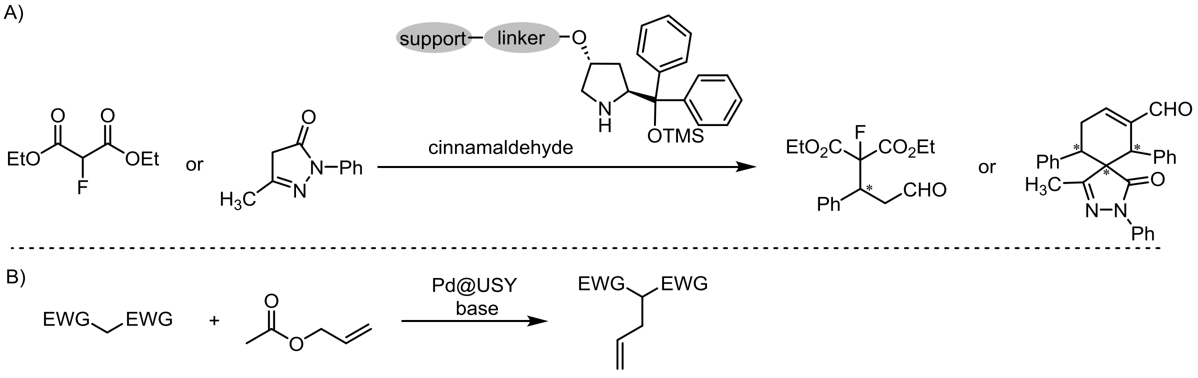
Homogeneous catalysis plays an important role in synthetic organic chemistry, enabling access to valuable molecules used across various fields of industry, including agrochemical, pharmaceutical, and material science. Despite its significant development, homogeneous organocatalysis still faces several challenges, such as the need for high catalyst loading, low stability under harsh reaction conditions, and poor recyclability. To address these limitations, considerable attention has been devoted towards strategies for transferring homogeneous catalysis into heterogeneous catalysis.[1]

Building on our previous work in both homogeneous[2] and heterogeneous[3] catalysis, we developed methods for the immobilization of chiral organocatalyst – specifically, Hayashi-Jørgensen analogue – as well as palladium nanoparticles on solid supports. The catalytic activity of the mesoporous silica-immobilized Hayashi-Jørgensen catalyst was evaluated in the stereoselective conjugate addition of fluoromalonate to cinnamaldehyde, as well as in the spirocyclization reaction of pyrazolone with cinnamaldehyde (Scheme 1A). Additionally, zeolite-impregnated palladium nanoparticles were successfully applied in the Tsuji-Trost allylic alkylation reaction using various carbon nucleophiles, such as malonate and oxoester derivatives, with allyl acetate (Scheme 1B).



Scheme 1: Application of A) immobilized organocatalysis in conjugated addition reactions and B) impregnated palladium nanonparticles in the Tsuji-Trost allylic alkylation.

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The formation of monetite on the synthesis and dehydration of brushite

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Calcium phosphates (CaPs) are a class of minerals with a significant number of studies involving its applications in medicine, water treatment, catalysis, and agriculture. Brushite, or dicalcium phosphate anhydrous (DCPD, $CaHPO_4.2H_2O$) and monetite, or dicalcium phosphate anhydrous (DCPA, $CaHPO_4$) are the CaPs with lowest Ca/P molar ratio, which makes them the more acidic and soluble phases. However, brushite is layered by the water molecules in its structure, while monetite is not, so their chemical and physical properties are distinct. Monetite is the dehydrated phase of brushite and both method synthesis are usually similar, with the addition of heat to favor monetite by avoiding the formation retention of water in the structure. In fact, monetite can be synthesized by heating brushite at high temperatures, causing its dehydration to its anhydrous phase, monetite. It has been observed in the literature the decomposition of brushite to monetite when heated in dry air at or above 45 °C, or heated in deionized or distilled water at or above 40 ºC[1]. The synthesis of brushite in this work involves the use of an hydrocalumite mother solution, mixed with a phosphate buffer solution (pH 6,8; $H_2PO_2^-/HPO_2^{2-}$) at different Ca/P ratios, and reaction temperatures. The brushite powders were analysed with X-Ray Diffraction (XRD) and are being reanalysed after periodical times to investigate its dehydration, even when stored at room temperature. It has been observed the formation of monetite from brushite depending on the reaction conditions. Temperatures above 35 °C and excess of calcium ions in the reaction system have shown to favor this behavior (Figure 1a). The reanalysis within 1 and 2 months showed a slow and gradual definition of monetite peaks. The process of dehydration is different from brushite powders synthesized in different reaction conditions. The sample produced molar ratio of Ca/P=1 has already shown defined monetite peaks within 1 month (Figure 2) and a significant decrease in the brushite peaks. It also shows peaks identified as hydroxyapatite (HA, $Ca_{10}(OH)_2(PO_4)_6$). Further investigation is needed to understand those behaviors.

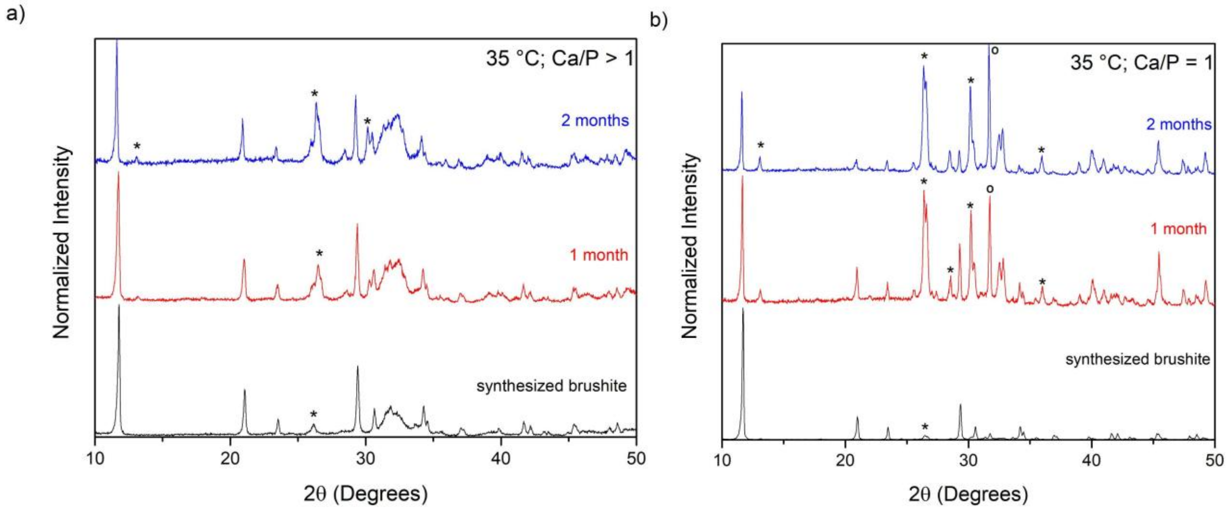

Figure 1: X-ray diffractograms of synthesized brushites with a) Ca/P molar ratio > 1 and the reanalysis within 1 and 2 months and b) Ca/P molar ratio = 1 and the reanalysis within 1 and 2 months. Monetite peaks are identified with * and hydroxyapatite peaks are identified with º.

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