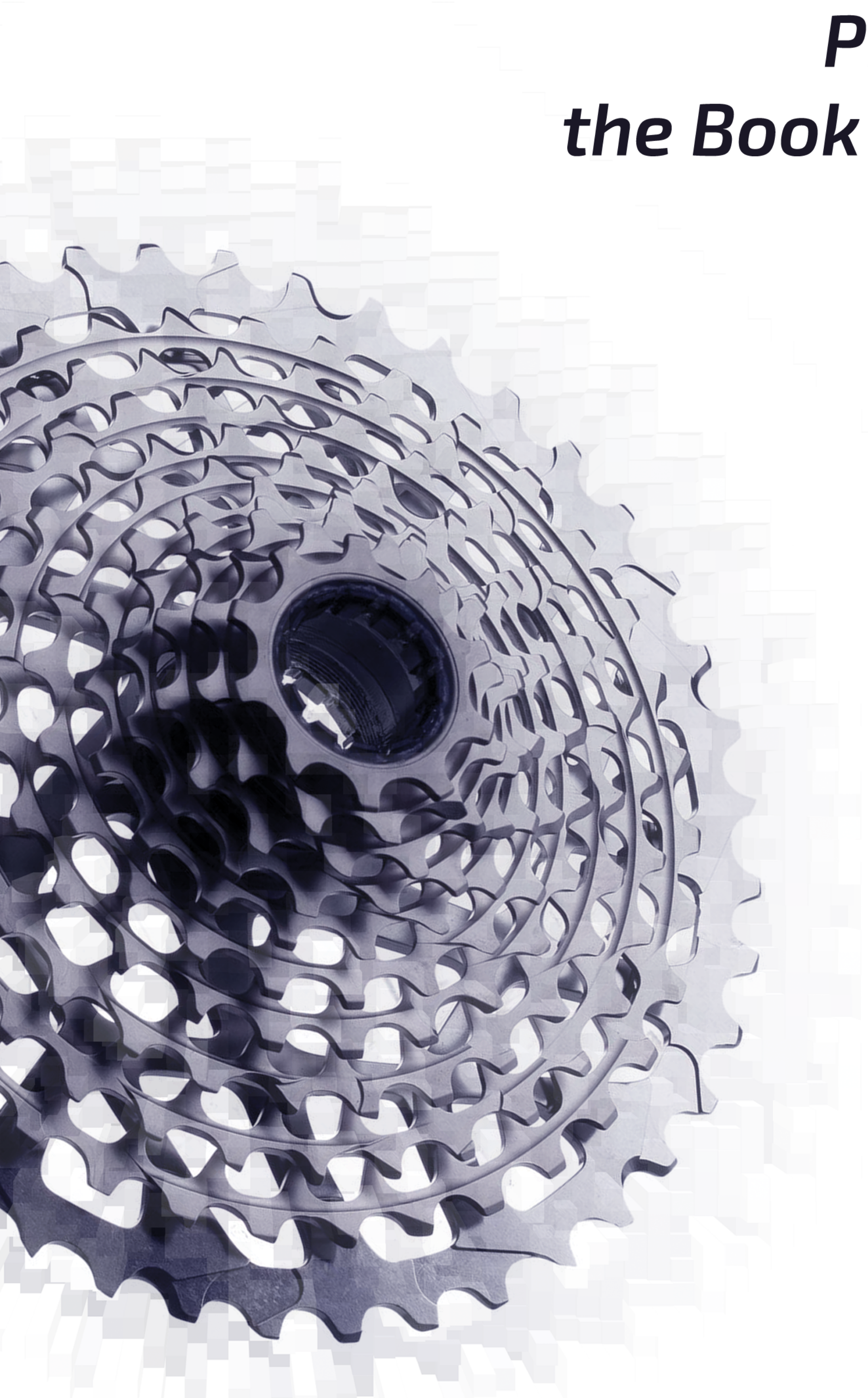
10th International Symposium on Materials for Energy Storage and Conversion

May 25th-28th, 2026 Belgrade, Serbia

Programme & the Book of Abstracts



HYDROGEN STORAGE INITIATIVE SERBIA
VINČA INSTITUTE of NUCLEAR SCIENCES - NATIONAL INSTITUTE of the REPUBLIC of SERBIA, UNIVERSITY of BELGRADE

PROGRAMME AND THE BOOK OF ABSTRACTS

10th International Symposium on Materials for Energy Storage and Conversion - mESC-IS 2026

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CONFERENCE PROGRAMME

Monday, May 25th 2026

8:30	Registration
9:00	Opening ceremony
SESSION 1	Chair: Marek Polanski
9:15	PLENARY LECTURE
	Jacques HUOT Development of High Entropy alloys for hydrogen storage
10:00	INVITED LECTURE
	Rezan DEMIR-ÇAKAN Design of Anode Materials for Practical Sodium-Ion Batteries: From Hard Carbon to Alloy Systems
10:25	**Emrah DEMIR** Soft-Hard Carbon Synergies for Sodium-ion Battery Anodes
10:40	**Kadir TÜRKMEN (online)** Tandem Copper - Cobalt Phthalocyanine Electrodes Enable Enhanced Electrochemical CO_2 Conversion to Ethylene
10:55	**Elif GÜLOĞLU (online)** Comparative Electrochemical Performance Analysis of NMC Cathodes Obtained from Recovered and Commercial Materials
11:10-11:25 **COFFEE BREAK**	
SESSION 2	Chair: Fabrice Leardini
11:25	INVITED LECTURE
	Marek POLANSKI Modern Alchemy: New Strategies for the Mechanochemical Synthesis of Solid-State Hydrogen Storage Materials
11:50	**Tomasz CZUJKO** MgH_2 morphological and structural changes during high-energy ball milling
12:05	**Vladislav ZADOROZHNYY** Effect of mechanical alloying and activation on the diffusion behavior and durability of metal hydride bulk materials
12:20	**Artem KOROL (online)** Comparison of residual stress values in TiFe alloy measured by $\sin^2\Psi$ and FIB-DIC techniques
12:35	**David Maria TOBALDI** Flexible 2D Layered Oxide Thin Films for Solid-State Hydrogen Storage

12:50 -15:00 **LUNCH BREAK**	
SESSION 3	Chair: Bojana Paskaš Mamula
15:00	INVITED LECTURE **Nong ARTRITH (online)** Harnessing Machine Learning for Advancing Amorphous Battery Materials
15:25	**Katarina BATALOVIĆ** From vast MXene design space to synthesizable MXENE/PANI composites: embedding guided, model driven interface engineering
15:40	**Çağatay YILDIZ (online)** Influence of convex enclosure structure on thermal discharge process of PCM
15:55	**Branislav STANKOVIĆ** Liquid-Assisted Mechanochemical Formation of $CsCuCl_3$: Insights from Machine Learning Potentials and DFT
16:10	**İdil KIVANÇLI** Electrochemical Noise as a Direct Probe for Copper Deposition Uniformity

Tuesday, May 26th

SESSION 4	Chair: Dragana Jugović
9:30	PLENARY LECTURE **Vojislav STAMENKOVIĆ** Progress on Electrochemical Interfaces for PEM Fuel Cells
10:15	INVITED LECTURE **Fabrice LEARDINI** Advanced metal chalcogenide electrocatalysts for hydrogen production by water splitting
10:40	**Sevinj JAVADOVA** Illumination-Dependent Electrochemical Impedance Analysis of Bi_2O_3-Based photoelectrodes
10:55	**Marko JELIĆ** Tailoring Surface Chemistry of Ni and Co overlayers on $BiVO_4$ Thin Films for enhanced solar fuel production
11:10	**Nikoloz NIORADZE** Nickel doped rice husk activated carbon composites: Potential electrodes in H_2 generation
11:25 -11:40 **COFFEE BREAK**	
SESSION 5	Chairs: Sanja Kurko & Tijana Pantić

11:40	INVITED LECTURE
	Eli GLIGOROVA Mg_2Ni based materials for hydrogen storage
12:05	**Grigor TATISHVILI** The importance of quantum mechanical models to explain hydrogen evolution
12:20	**Gülhan ÇAKMAK** Design of Composite SOFC Cathodes via Spray Pyrolysis: Synergistic Effects of Perovskite and Ruddlesden–Popper Phases
12:35	**Lela KIVNIKADZE** Shaping Georgia’s Green Hydrogen Transition: a Socio-Technical Triad Approach
12:50 **LUNCH**	
20:00 **CONFERENCE DINNER** *Restaurant REKA*	

Wednesday, May 27th

SESSION 6	Chair: Jasmina Grbović Novaković
9:30	PLENARY LECTURE
	Mykhaylo LOTOTSKYY Features of energy storage and conversion technologies utilizing metal hydrides
10:15	INVITED LECTURE
	Fusheng YANG Recent developments on metal hydride hydrogen compressors-A comprehensive review

10:40	INVITED LECTURE
	Nikola BILIŠKOV Solid-state reactions – what we already see and what else we would like to see
11:05	**Aybaniz AHADOVA** (online) Isothermal decay analysis of quartz
11:25 -11:40 **COFFEE BREAK**	
11:40	**“NO DEPENDENCE” PROJECT MEETING** For project participants
12:40 **LUNCH BREAK**	
15:00	*Forum* **Gender Dynamics in Science and Energy** Institut francais

16:00 – 18:00	**POSTER SESSION** **CLOSING REMARKS** Institut francais
Thursday, May 28th	
11:00	**Excursion to Novi Sad** Lunch and wine tasting in Winery KOVAČEVIĆ

POSTER PRESENTATIONS

P1	Nada Adamović	A1	Waste-Derived Powellite: Structural Aspects and Energy Storage Potential
P2	Ramiz Gultekin Akay	A3	Investigation of Degradation in Functionalized h-BN/PBI Composite Membranes for HT-PEMFCs
P3	Tanja Asanovic Antonic	A5	Linking Phase Stability and Oxygen-Vacancy Energetics in High-Entropy Oxide Nanofibers via Machine-Learned Potentials
P4	Gozde Atac	A6	Electrochemical Noise Analysis Coupled with EIS Interpretation in Li/MnO_2 Primary Batteries
P5	Şebnem Cingisiz-Uygun	A9	Practical High Energy Na-Ion Batteries with Sn-Based Composite Anodes
P6	Jasmina Grbović Novaković	A11	Development of Hydrogen Compressors
P7	Jelena Jovanović	A15	Sustainable Rare Earth Recovery Using Nicotinium-based Ionic Liquid Polymer Inclusion Membranes
P8	Dragana Jugović	A16	Polymorphism and Transition Metal Doping in $NaFeO_2$-Based Cathodes
P9	Sandra Kurko	A19	MoS2/Polypyrrole composites as electrocatalysts for Hydrogen Evolution Reaction
P10	Bojana Kuzmanović	A20	Synthesis and Optimization of $Ti_3C_2T_x$ MXene Materials and Their Integration into PANI/MXene Composites
P11	Lela Kvinikadze	A21	Shaping Georgia’s Green Hydrogen Transition: a Socio-Technical Triad Approach

P12	Snežana Lazić Knežević	A22	Deterministic Cost-Effective Strain Engineering of Quantum Light Emitters in Two Dimensional Semiconductors
P13	Mirjana Medić Ilić	A23	Ag and Fe Alloying in Mg_2Ni Systems: Impact on Surface Composition and Corrosion Behavior
P14	Sanja Milošević Govedarović	A24	Desorption kinetics from MgH2-W composites
P15	Tijana Pantić	A26	X-ray Absorption Spectroscopy Study of Mg-V Thin Films for Hydrogen Storage
P16	Bojana Paskaš Mamula	A27	Computational Screening of Li and Na Amidoborane Formation
P17	Milica Prvulović	A28	Catalytic Effects of Ni and Co on MgH2 Hydrogen Desorption under Short Milling Times
P18	Jana Radaković	A29	Machine learning-assisted, literature-based screening of high-entropy alloys for solid state hydrogen storage
P19	Ivana Radisavljević	A30	Effects of 3d metal doping on local and electronic structure of CeO2 nanopowders
P20	Zilong Wang	A36	Optimal control on a single stage metal hydride hydrogen compressor: A Pontryagin minimization approach
P21	Aygün Zeynalova	A41	The influence of the composition of Ni-P thin films on their electrocatalytic properties
P22	Šaban Žuna	A42	The Role of Hydrogen in the HDH Process for Producing Titanium Alloy Powder for Additive Manufacturing

PLENARY LECTURES

Development of High Entropy alloys for hydrogen storage

Jacques Huot [1], Salma Sleiman [1], Gregue Céruthi Tsoumou [1]

1 Université du Québec à Trois-Rivières, Trois-Rivières, Québec, G8Z 4M3, Canada

doi: 10.5937/MESCIS26001H

Recently, high entropy alloys (HEA) have been investigated for hydrogen storage applications. In this talk we will review some characteristics of HEA that have an impact on the usefulness of HEA for practical applications. One of the key factors in determining the price of a metal hydride is the conditions of the first hydrogenation. We will show the impact of particle size, temperature and hydrogen pressure on the first hydrogenation on the TiVZrHfNb HEA. Figure 1 shows that the incubation time of the first hydrogenation is strongly dependent on temperature [1].

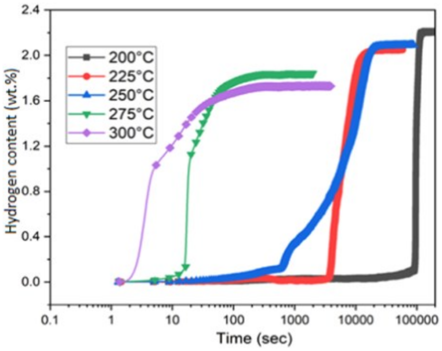

Figure 1. First hydrogenation kinetics of TiVZrHfNb alloy particles of 0.5 mm under 20 bars of hydrogen pressure.

By plotting the incubation time as a function of 1/T, we found that the incubation time follows the Arrhenius mechanism with an activation energy of 241 kJ/mol H_2.

Usually, a HEA should have a BCC (Body Centred Cubic) structure in order to be able to absorb hydrogen. However, upon the substitution of elements, a second phase could be present. We will present the effect of substituting titanium by zirconium in the system $Ti_{20-x}Zr_xV_{35}Cr_{15}Ni_{10}Mn_{20}$ (x = 0, 4, 8, 12, 16 et 20). This substitution was chosen because zirconium having a bigger atomic radius, the possibility of the appearance of a Laves phase is higher. The diffraction patterns, presented in figure 2, show that the proportion of Laves phase increases with increasing x.

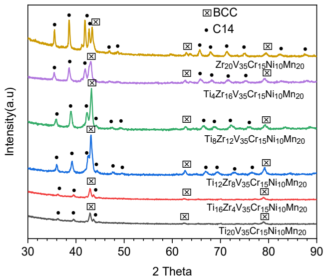

Figure 2. Diffraction patterns of as-cast alloys $Ti_{20-x}Zr_xV_{35}Cr_{15}Ni_{10}Mn_{20}$ (X=0, 4, 8, 12, 16, and 20).

We also found from neutron diffraction that, in the Laves phase, elements occupy specific atomic positions.

All of these alloys readily absorbed hydrogen at room temperature without any prior treatment. The fast first hydrogenation is due to a synergetic effect between the BCC and Laves phase in these alloys [2]. This synergetic effect was further investigated for the alloy $Ti_{16}Zr_4V_{35}Cr_{15}Ni_{10}Mn_{20}$ by casting separately the BCC and the C14 phases. It was found that, individually, the BCC and Laves phases do not absorb hydrogen in their as-cast state. Hydrogenation is possible only after a short milling time. Figure 3 shows the first hydrogenation kinetics of the parent alloy ($Ti_{16}Zr_4V_{35}Cr_{15}Ni_{10}Mn_{20}$) along with the kinetic of the C14 and BCC phases milled together and also the sum of the individual BCC and C14 kinetics.

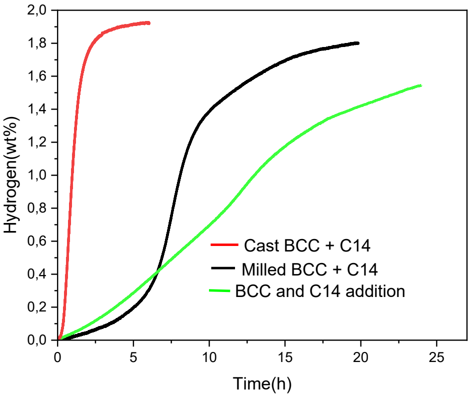

Figure 3. First hydrogenation kinetics at room temperature and 2000 kPa of hydrogen of as-cast $Ti_{16}Zr_4V_{35}Cr_{15}Ni_{10}Mn_{20}$ alloy along with C14 and BCC individual phase kinetics.

We see that milling both phases together improves the kinetic, but it is still much slower than when both phases are cast together. This is a proof that a synergy between the Laves phase and the BCC phase is essential for a fast and complete hydrogenation.

References

[1] S. Sleiman and J. Huot, Journal of Alloys and Compounds 861 (2021) 158615. https:// doi.org/10.1016/j.jallcom.2021.158615

[2] G.C. Tsoumou and J. Huot, International Journal of Hydrogen Energy 206 (2026) 153384. https://doi.org/10.1016/j.ijhydene.2026.153384

Professor Huot has a Ph.D. in physics. He did a postdoc in Japan under the supervision of Professor Etsuo Akiba where he started working on metal hydrides. From 1995 to 2004, Professor Huot was a researcher at Hydro-Québec where he studied magnesium-based nanocrystalline alloys for hydrogen storage. Since 2004 he is a professor at UQTR and a member of HRI. His expertise is solid-gas interactions, metal hydrides, and material characterization. He published 250 papers and is a co-inventor of 10 patents.

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Features of energy storage and conversion technologies utilizing metal hydrides

Mykhaylo Lototskyy [1,2], Boris Tarasov [2], Volodymyr Yartys [3,4]

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Hydrogen and renewable energy sources play a key role in a clean transition to zero-emission energy, transportation and industry. Metal hydrides (MH) are one of the most promising groups of materials assisting in realization of this strategy.

Reversible formation/decomposition of MHs involves two mechanisms (Figure 1): the interaction of the parent metal/intermetallic compound with H_2 gas (Eq. 1) and electrochemical hydrogenation of the metal (or hydride decomposition) in an electrolyte, e.g., aqueous alkaline solution (Eq. 2). Accordingly, the applications of MHs can be generally classified as the gas-phase [1] and electrochemical [2].

$$\mathrm{M}\ (s) + x/2\ \mathrm{H_2}\ (g) \leftrightarrow \mathrm{MH_x}\ (s) + \mathrm{Q}; \qquad (1)$$

$$\mathrm{M}\ (s) + x\ \mathrm{H_2O}\ (l) + e^- \leftrightarrow \mathrm{MH_x}\ (s) + \mathrm{OH^-}\ (l); \qquad (2)$$

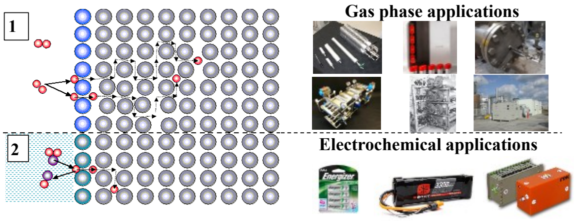

Figure 1. Gas-phase and electrochemical applications of metal hydrides.

Extremely wide range of thermodynamic stabilities of MHs depending on their composition allows for their use in various applications which significantly differ in the operating conditions (Figure 2).

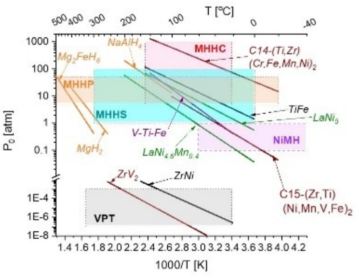

Figure 2. Van't Hoff plots of some MH materials vs. applications: VPT – vacuum-plasma technologies (getters and low-pressure sources of H isotopes), MHHS – MH H_2 storage systems, MHHP – MH heat management systems, MHHC – thermally driven MH H_2 compressors, NiMH – Ni-MH batteries.

Most of the MH applications are very important for energy storage and conversion technologies. The gas-phase applications allow to combine the processes of compact and safe hydrogen storage and its supply, along with the utilization of waste heat released during operation of other system components. Direct storage of electricity is provided by electrochemical applications of MHs.

This presentation analyzes impact of main properties of MH materials on the system performance in the relevant applications. The focus is put on the thermodynamics of H–M interaction as a main factor which determines suitability of the MH material to the application conditions (operating temperatures and H_2 pressures or electrochemical potentials). Other features include structure and morphology, hydrogenation/dehydrogenation kinetics, cycle stability and tolerance to impurities.

Thus, MH material properties are the key factors defining the development of any application of metal hydrides, and the general strategy of the system development should realize the down-top approach "From material to system" when the first stage includes a comprehensive studies of various properties of the selected MH material followed by the development of the MH reactor and its integration in the end-use hydrogen energy systems. At the same time, selection criteria of the MH materials should account for the conditions of their use in specific applications (see Figure 3). The talk will present important examples of such applications and will discuss the properties of the relevant optimized hydrides.

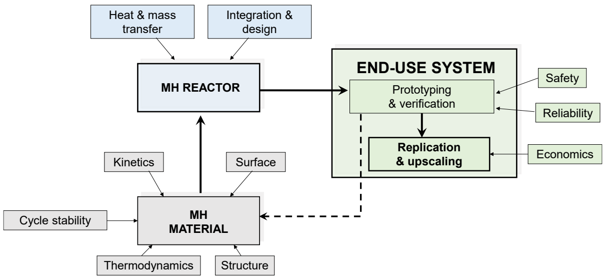

Figure 3. R&D strategy in the implementation of MH technologies

References

[1] M.V. Lototskyy, B.P. Tarasov, V.A. Yartys, J. Energy Storage (2023) 1081658. https://doi.org/10.1016/j.est.2023.108165

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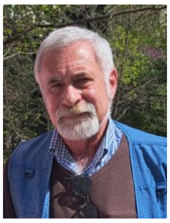

Dr Mykhaylo Lototskyy is an internationally recognized researcher in hydride materials science and applications of metal hydrides (159 Scopus-indexed publications cited more than 9000 times since 1985; h=49). Presently, he is a Key Program Manager at HySA Systems Centre of Competence in South Africa and Head of Laboratory of Metal Hydride Energy Technologies at FRC PCP&MC RAS in Russia.

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Progress on Electrochemical Interfaces for PEM Fuel Cells

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University of California, Irvine

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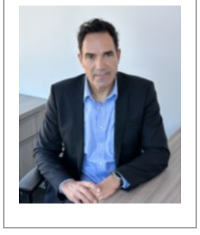
Electrochemical energy conversion and hydrogen production, such as fuel cells and electrolyzers have evolved as a prevailing option in achieving environmentally neutral energy, including transportation sector. Global deployment of these technologies dictates perpetual demand for improved functionality and performance of employed materials that are mainly based on scarce elements. Research aimed towards the design and synthesis of materials with advanced electrochemical properties, while diminishing the need for rare constituents, will be presented. Emphasis will be placed on the fundamental understanding of well-defined electrified interfaces and resolving their functionality at atomic and molecular scale and how they are related to device performance. The role of surface structure, spatial arrangement and nature of the employed elements will be presented for the cathodic reaction through the challenges that are being addressed, including technical targets and barriers for PEM fuel cells.



Vojislav Stamenković is a Professor at the University of California, Irvine, Department of Chemical and Biomolecular Engineering. He is also the founding Director of Horiba Institute for Mobility and Connectivity at the UCI's Henri Samueli School of Engineering.
He serves as an Associate Editor at ACS Catalysis, and on the Editorial Board of Surface Science and Surface Science Letters.

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INVITED LECTURES

Harnessing Machine Learning for Advancing Amorphous Battery Materials

Nong Artrith

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doi: 10.5937/MESCIS26004A

Many materials with applications in energy, e.g., batteries, are non-crystalline or exhibit complex chemical disorder and multicomponent compositions. This complexity makes direct modeling with first-principles methods challenging. To address this challenge, we developed accelerated sampling strategies based on machine learning interatomic potentials (MLIPs), genetic algorithms, and molecular dynamics simulations [1]. Here, I will discuss the methodology and its applications to both amorphous and crystalline battery materials. For amorphous materials, we constructed the phase diagram of LiSi alloys, which are prospective anode materials for lithium-ion batteries [2], and mapped the composition-structure space of lithium thiophosphate (LiPS) solid electrolytes [3-5], correlating thermodynamic stability and ionic conductivity with local structural motifs to identify structure-composition-property relationships. For crystalline layered oxides, our recent work demonstrates the use of MLIPs for direct atomistic simulations of $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811), enabling efficient and accurate prediction of Li-ion transport properties that would be computationally prohibitive with conventional first-principles methods. Complementing these simulations, X-ray absorption spectroscopy (XAS) provides local chemical insights; we established an S/P/O Kedge XAS databases for LiPS / NMC811 materials using simulated structures [3]. Together, these studies illustrate how ML-driven simulations integrated with spectroscopic analysis can accelerate the understanding and design of complex battery materials at the atomic scale.

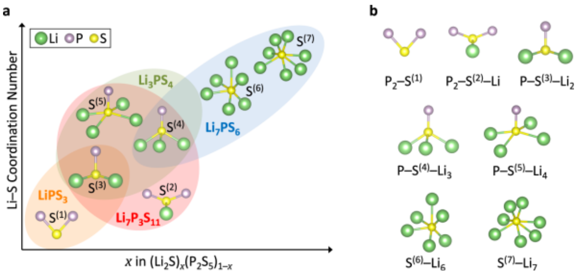

Figure 1: Schematic illustration [4] of the local coordination of S atoms with Li and P atoms in selected (Li2S)x(P2S5)1–x crystalline structures. Li: green; S: yellow; P: purple. LiPS3: orange region; Li7P3S11: red region; Li3PS4: green region; Li7PS6: blue region.

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[1] N. Artrith and A. Urban, *Comput. Mater. Sci.* **114**, 135-150 (2016).

[2] N. Artrith, A. Urban, and G. Ceder, *J. Chem. Phys.* **148**, 241711 (2018).

[3] H. Guo, Q. Wang, A. Urban, and N. Artrith, *Chemistry of Materials* **34**, 6702-6712 (2022).

[4] H. Guo, M.R. Carbone, C. Cao, N. Artrith, A. Urban, D. Lu, et al, *Scientific Data* **10**, 349 (2023).

[5] C. Cao, M.R. Carbone, C. Komurcuoglu, S. Jagriti, N. Artrith, A. Urban, D. Lu, F. Wang et al, *Cell Reports Physical Science,* **5**, 101909 (2024)

Nong Artrith is a tenured Assistant Professor in the Materials Chemistry and Catalysis Group at the Debye Institute for Nanomaterials Science, Utrecht University (and was a Visiting Researcher at Microsoft Research Amsterdam Lab 2022-2023). Nong was a Research Scientist at Columbia University, USA, and a PI in the Columbia Center for Computational Electrochemistry. Her research interests focus on the development and application of first principles and ML methods for the computational discovery of energy materials and for the interpretation of experimental observations.

Presenting author: Nong Artrith **e-mail:** n.artrith@uu.nl

Solid-state reactions – what we already see and what else we would like to see?

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1 Ruđer Bošković Institute, Zagreb, Croatia

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Claiming that any chemical reaction requires mobility of reactant molecules to allow their collisions sounds straightforward and self-explanatory. Indeed, this fundamental principle is inherently satisfied in fluidic states of matter. However, chemical reactions evidently take place in the solid state, which is relatively easily understood for amorphous solids, but chemical reactions readily happen even between crystalline reactants. This, at least apparently, challenges our idea of the solid (crystalline) state as a collection of immobile atoms, ions or molecules. Obviously, it is hard to imagine that two well-ordered assemblies of particles productively interact to produce a third well-ordered assembly. However, things start to become clearer if we imagine a metastable intermediate state, taking place on the way from reactants to products. If amorphous, such a state facilitate mobility of the reacting species, making the reaction possible.

Indeed, techniques that enable time-resolved in-situ monitoring of solid-state chemical processes regularly reveal the appearance of amorphous, in the extreme examples even fluid intermediates preceding development of final product. Thus observed amorphous phases play an active role at the first stages of solid-state reactions. Techniques for in-situ monitoring of mechanochemical reactions are now well established, but they continue to develop, constantly introducing new methods and approaches.

On the other hand, it is clear that solid-state chemical reactions are initiated by the contact of two substances and take place on the interface. Although theoretically considered over a long period of time, starting with the publications of J. W. Gibbs, this fundamental aspect has not been experimentally dealt with in sufficient detail so far. However, it is clear that a detailed understanding of the processes in the zone around the solid-solid interface reveal fundamental aspects of solid-state reactivity in general. Different to mechanochemical reactions, solid-state contact reactions should be dominantly driven by diffusion of the reactants through the interface and their productive combination in the reaction zone.

Summary, a comparative analysis of the same solid-state reactions performed in drastically different conditions (mechanochemical vs. contact reaction) could give important insights into the mechanistic details by resolving specific contributions. In line with this, a large number of chemical reactions, ranging from inorganic (metatheses, complexations, redox reactions etc.) to organic (cocrystallizations, covalent bond forming reactions etc.) were monitored in their macrtoscopically static (contact reaction) and macropically dynamic (mechanochemical) versions. This comparative study enables a resolution of kinetic and other parameters that determine overall solid-state reactivity.

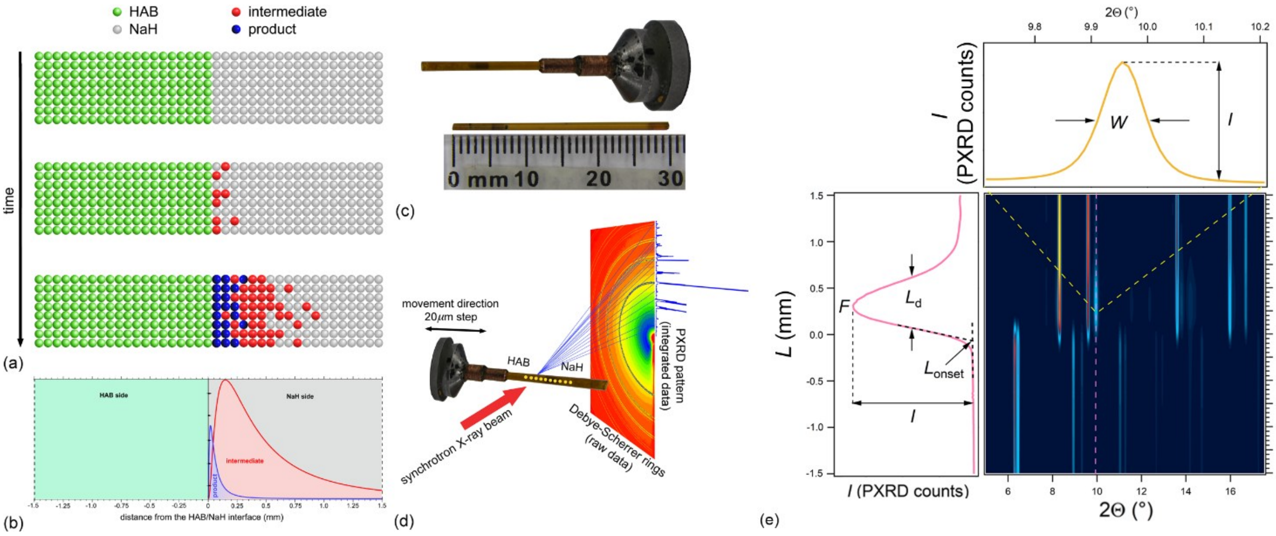

Figure 1 Reaction on the solid-solid interface (NaH + NH_3BH_3 in this example). (a) scheme of the interdiffusion of the reactants and chemical processes in the reaction zone around the interface with (b) the expected reaction profile. The reaction is performed in capillary (c), half-filled with reactant A and reactant B on the opposite side, brought to contact on the interface. The reaction is mapped by synchrotron X-ray powder diffraction (d) step-by-step at predefined positions with respect to the interface. (e) Representation of the obtained data, parameters derived parameters from PXRD patterns of a particular component (in this case product) of the system.

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Design of Anode Materials for Practical Sodium-Ion Batteries: From Hard Carbon to Alloy Systems

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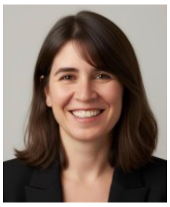
Sodium-ion batteries (NIBs) are emerging as promising alternatives to lithium-ion systems due to low cost, safety, and resource abundance, but their energy density is still limited by the performance of electrode materials. This talk focuses on the rational design of anode materials, starting from hard carbon, which remains the most practical option but is still challenged by limited capacity and complex Na-storage mechanisms. To accelerate material optimization, a machine learning (ML)-guided approach is introduced, linking synthesis conditions, structural features, and electrochemical performance to identify key descriptors governing sodium storage behavior. This data-driven framework enables faster and more efficient optimization of carbon anodes. Finally, the discussion extends to alloy-type anodes, which offer higher theoretical capacities but suffer from large volume changes. Strategies combining structural engineering and interface stabilization are presented within a unified rational design perspective for next-generation Na-ion battery anodes.



Rezan Demir-Cakan received her Ph.D. degree in 2009 from the Max Planck Institute of Colloids and Interfaces. She is currently a Professor in the Department of Chemical Engineering at Gebze Technical University. Her research activities center on the design and synthesis of nanostructured energy materials for advanced battery systems, with particular emphasis on sodium-ion, lithium–sulfur, and aqueous electrolyte zinc-ion batteries.

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Mg_2Ni based materials for hydrogen storage

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Mg-based materials have some important advantages as hydrogen storage media as light weight, high theoretical absorption capacity, good reversibility, abundance and low coast. They also have some drawbacks as slow hydrogen sorption kinetics and high sorption temperatures that can be overcome by different additives combined with high energy ball milling under argon or hydrogen and partial substitution. Using different carbon compounds, ball milled with Mg /MgH_2 or Mg_2Ni, lead to reduction of hydrogen sorption temperature, improved kinetics and also prevented particles growth upon milling and repeated hydrogen absorption and desorption. Mg_2Ni is a highly promising solid-state hydrogen storage material with a 3.6 wt. % theoretical hydrogen storage capacity. Its primary advantages include lower desorption temperatures 250- 300°C and faster kinetics compared to pure magnesium. The nanoporous activated carbons used in this study is prepared by hydropyrolysis processing from precursor polyolefin wax (POW) which is a polyethylene production waste. This nanocarbon is distinguished by high surface area and prevailing microporous structure. The other two prepared materials have composition $Mg_{1.7}Ni_{0.7}Ti_{0.3}Co_{0.3}$ and $Mg_{1.85}Ni_{0.85}Ti_{0.15}Co_{0.15}$. The 2 wt.% of obtained carbon POW and 98 wt.% $Mg_{2.1}Ni$ mixture is prepared by ball milling in a planetary mill under Ar for 30 h. The other two Mg_2Ni based materials are prepared also via ball milling under argon for 3 hours. The mixture of corresponding compositions of powdery Mg, Ni, Co and Ti are ball milled in a planetary monomill Fritsch Pulverisette 6 is under argon with rotation speed 300 rpm and 1:10 sample to balls weight ratio. Structure and phase composition are monitored by XRD analyses and after ball milling and hydrogenation by TEM (TEM HR STEM JEOL JEM 2100). Through the Image J program, the histograms of the distribution of particle size for all samples are done. TEM characterization of these materials is challenging, because of their sensitivity to oxidation and the high energy of the electron beam exposure, which could cause negative impact on them so the HRTEM and SAED were obtained by low beam current values. The hydrogen absorption and desorption measurements are performed by Sivert's type apparatus. Hydrogenation was proceeded at 300^0 C and 200^0 C and P= 1 MPa and dehydrogenation at 300^0 C and P = 0.15 MPa. The SAED and HRTEM revealed that the materials consist of mainly Mg_2NiH_4 with monoclinic and orthorhombic structures and MgH_2, but also some traces of Mg, Ni and MgO and some graphitic structure areas. The 98 wt. % $Mg_{2.1}Ni$ – 2 wt.% POW showed hydrogen absorption capacity value of 3.3 wt.% after 1h of hydrogenation at 300^0C and 1 MPa. The $Mg_{1.7}Ni_{0.7}Ti_{0.3}Co_{0.3}$ and $Mg_{1.85}Ni_{0.85}Ti_{0.15}Co_{0.15}$ reached 2.8 wt. % and 3.2 wt.% of hydrogen absorption capacity at the same temperature and pressure. The investigated materials showed very fast kinetics of absorption at 300^0 C and 200^0 C and 1MPa. The desorption for all three samples is fast, but proceeded at 300^0 C and 0.15 MPa. The composition of $Mg_{2.1}Ni$ and nanoporous carbon derived from POW has more pronounced positive effect on absorption kinetics of MgH_2, because of the formation of Mg_2NiH_4 and the high pore volume and specific surface area of this nanocarbon.

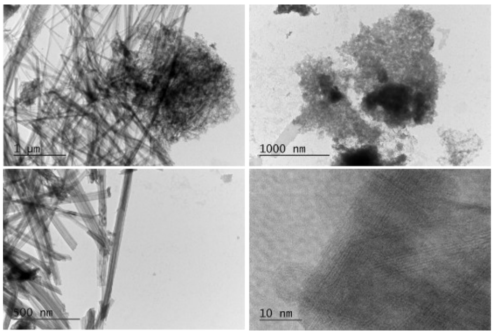

Figure 1. HRTEM images of various carbon structures in prepared POW: turbostratic graphite, fullerene-like carbon, nanodiamond, carbon onion, graphite ribbons , CNTs, barrel-like particles, and ordered graphite.

Using nanocarbon derived from polyethylene production waste polyolefin wax, as additive to $Mg_{2.1}Ni$, leads to the production of hydrogen storage materials with higher capacity and better kinetics than these with composition $Mg_{1.7}Ni_{0.7}Ti_{0.3}Co_{0.3}$ and $Mg_{1.85}Ni_{0.85}Ti_{0.15}Co_{0.15}$.

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Advanced metal chalcogenide electrocatalysts for hydrogen production by water splitting

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The rational design of advanced electrocatalysts for hydrogen production using water and electrical energy supply from renewable sources is a critical issue that must be addressed to promote the energy transition. At the Materials of Interest in Renewable Energies (MIRE) group at Universidad Autonoma de Madrid we work on the growth and characterization of metal chalcogenides to be used as electrodes (or photo-electrodes) in water splitting devices. Among these compounds we have investigated transition metal chalcogenides, such as TiS_3 [1] or highly defective ultrathin MoS_2 nanocrystals [2].

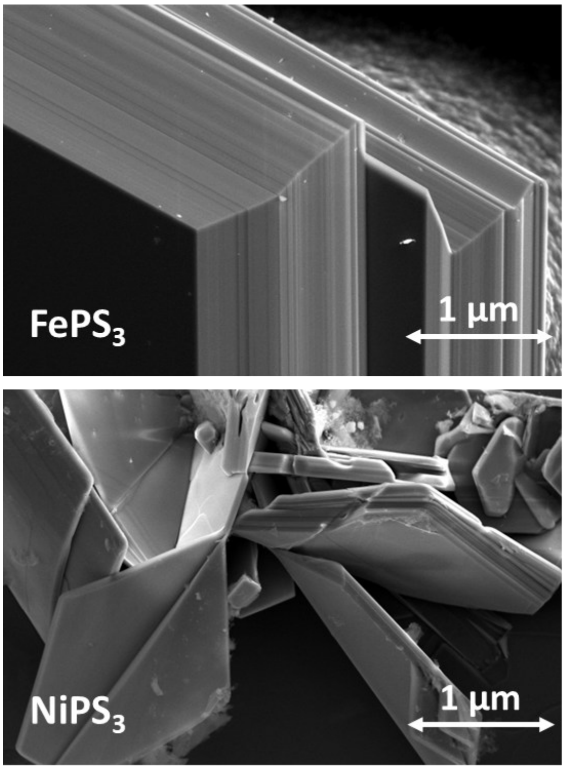

Figure 1. Scanning electron micrograph of $FePS_3$ and $NiPS_3$ flakes showing their layered morphology.

Recently we have also focused on metal phosphorous trisulfides, which have shown excellent properties as electrodes for water splitting [3]. I will present original results on the preparation and characterization of $Fe_xNi_{1-x}PS_3$ (x=1, 0.25, 0.5, 0.75, and 0) mixed phases. These compounds have been prepared by chemical vapor transport and characterized using a plethora of techniques, such as X-ray diffraction, scanning electron microscopy (Fig.1), energy-dispersive X-ray spectroscopy, electron photoemission spectroscopy, Raman spectroscopy, and optical transmission spectroscopy. Finally, electrodes were prepared via mechanical exfoliation [4] and using them as anodes for the oxygen evolution reaction in alkaline electrolytes. The main results obtained by MIRE group with these chalcogenides will be presented and discussed from the perspective of their use as electrodes for water electrolysis.

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Modern Alchemy: New Strategies for the Mechanochemical Synthesis of Solid-State Hydrogen Storage Materials

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Mechanochemical synthesis has emerged as a powerful route for the preparation of solid-state hydrogen storage materials; however, conventional room-temperature ball milling approaches remain limited by kinetic constraints, restricted reaction pathways, and insufficient control over thermodynamic parameters. In this work, a set of advanced mechanochemical strategies referred to as “modern alchemy” is presented, aimed at extending the capabilities of mechanochemistry and enabling the synthesis of next-generation hydrogen storage systems.

The study focuses on unconventional processing conditions, including high-temperature and high-pressure reactive milling (up to 450°C and 100 bar H_2), enabled by a dedicated reactor design [1]. These conditions allow direct coupling of mechanical activation with thermodynamic driving forces, significantly accelerating reaction kinetics and enabling the formation of phases inaccessible under standard conditions. At the same time, it is demonstrated that excessive thermal input may negatively affect phase selectivity in more complex systems, highlighting the need for precise process control [2]. Complementary approaches such as cryogenic milling (−196°C) are introduced to enhance defect generation and suppress diffusion-driven coarsening, leading to improved reactivity. In parallel, alternative feedstock strategies are explored, including the use of metallic wires instead of powders, which offers a cost-effective route for processing high-value materials and introduces unique deformation mechanisms. The concept of “alloying of already alloyed” systems is also examined, enabling modification of intermetallic compounds through secondary mechanochemical processing. A notable aspect of this work is the use of unconventional substrates, such as stainless steel, as reactive components in synthesis. This approach enables the formation of multicomponent hydrogen storage materials with remarkably low hydrogen absorption temperatures, challenging traditional assumptions regarding contamination effects [3]. A key breakthrough is the development of self-shearing reactive milling under hydrogen atmosphere. This method enables spontaneous hydrogenation at room temperature through continuous surface renewal, even in the absence of grinding media. The approach is demonstrated for FeTi and extended to titanium-based alloys, effectively overcoming activation barriers without the need for alloying additives or high-temperature treatment [4]. To accelerate materials discovery, combinatorial milling is introduced, allowing simultaneous synthesis of multiple compositions [5]. This is supported by numerical modeling (DEM) and experimental observations of ball dynamics, providing insight into energy transfer and reaction mechanisms. Additionally, passive thermal management strategies are proposed to stabilize processing conditions and improve reproducibility.

Overall, the presented framework demonstrates that mechanochemistry can be transformed into a highly tunable and design-driven synthesis methodology. By integrating controlled thermodynamic conditions, innovative feedstock concepts, and novel reaction mechanisms, this work opens new pathways for efficient and scalable synthesis of advanced hydrogen storage materials.

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Recent developments on metal hydride hydrogen compressors - A comprehensive review

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Metal hydride hydrogen compressor (MHHC) utilizes the difference in hydrogen absorption/desorption equilibrium pressures of hydrogen storage alloys at different temperatures as the thermodynamic driving force to convert low-grade heat directly into hydrogen compression work. Characterized by the absence of moving parts, excellent sealing performance, and high hydrogen purity, MHHC represent one of the most typical routes in non-mechanical hydrogen compression technology. Since Wiswall and Reilly proposed the principle of thermally driven hydrogen storage alloy compression in the 1970s, MHHC technology has undergone over half a century of development, accumulating substantial research outcomes in the screening of AB_5- and AB_2-type alloys, the construction of multistage reactor systems, and engineering demonstrations, with laboratory prototypes achieving outlet pressures exceeding 700 bar[1,2].

However, a critical review of existing literature reveals that the intrinsic linkages among the three main research strands-materials, reactors, and systems-remain notably weak. At the material level, alloy development has long relied on elemental substitution and experimental screening, focusing on parameters such as plateau pressure, hysteresis coefficient, and cyclic stability. A systematic logical framework is still lacking for inversely constraining material design based on the application requirements of specific temperature-pressure windows. At the reactor level, the introduction of heat transfer enhancement strategies generally presupposes a given material. Although structural optimization studies involving fins, metal foams, etc., are quite extensive, the constraining mechanisms of material pulverization behavior, bed expansion, and porosity evolution on reactor configuration selection have yet to be adequately incorporated into the design phase. At the system level, most existing performance models are built upon ideal PCT relationships; the effects of actual material state evolution during cycling and transient reactor thermal response on system output have not been effectively integrated into the evaluation framework. This fragmented, parallel advancement of the three research strands has resulted in a lack of a unified, cross-scale understanding of the mechanisms governing MHHC performance. This structural gap may be even more critical than performance deficiencies at any single scale.

Based on this assessment, this paper presents a systematic review of key research advances in the MHHC field, organized around the cross-scale coupling mechanism of "material-reactor-system." Through bibliometric analysis and keyword evolution analysis, we reveal the progressive shifting patterns of research foci in MHHC. Combined with a critical reexamination of milestone publications, we clarify the developmental trajectories and disconnections among the three research strands, thereby providing a foundation for the analytical framework of the review. Subsequently, we analyze, layer by layer, how factors at each scale constrain the actual compression performance of MHHC: from thermodynamic plateau characteristics, hydrogen absorption/desorption kinetics, and cyclic stability of compression materials; to heat and mass transfer, bed structure evolution, and configuration matching constraints at the reactor level; and finally, to interstage thermodynamic matching, operational pacing control, and efficiency boundaries at the system level.

This paper further proposes that engineering application-oriented MHHC research should be driven by the target application scenario (temperature range, pressure range, heat source conditions), take material thermodynamic and kinetic parameters as the starting constraints, use reactor structure–bed behavior matching as an intermediate bridge, and place system control and performance evaluation as the end goal. A collaborative design logic that integrates reverse constraints and forward validation across the three levels should be established. This paper aims to move beyond the conventional paradigm of discussing materials, reactors, and system control in parallel, and to reexamine the mechanisms governing MHHC performance from a cross-scale coupling perspective, offering a reference for transitioning the field from isolated performance optimization toward application-driven, systematic design.

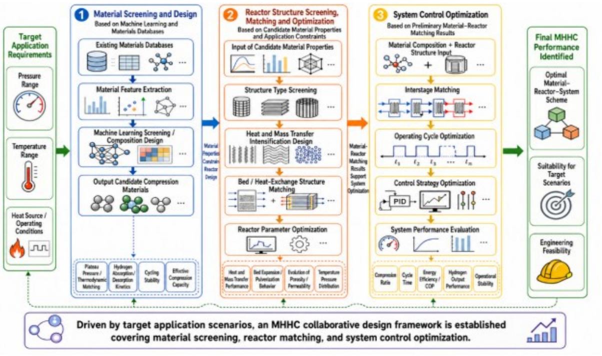

Figure.1 MHHC multi-scale collaborative design technical route for target scenarios.

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ORAL AND POSTER PRESENTATIONS

Waste-Derived Powellite: Structural Aspects and Energy Storage Potential

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There is a growing demand for low-cost and environmentally friendly materials for widely accessible energy storage devices. Within the $AMoO_4$ (A = Fe, Ca, Ni, etc.) family, $CaMoO_4$ (powellite) is distinguished by its favorable physical and chemical properties and its stable tetragonal crystal structure. Owing to these attributes, it has been widely explored as a functional material for applications in solid-state lighting, energy storage, temperature sensing, solar cells, and biomedicine [1–3].

In this study, a simple and cost-effective method for synthesizing a powellite ($CaMoO_4$)-based composite material with potential applications in capacitors as well as supercapacitors is presented. The main novelty of this research lies in the utilization of different waste materials for powellite synthesis. Specifically, waste $MoSi_2$ was fully reused and converted into a mixture of amorphous SiO_2 and MoO_3 through heat treatment at 500 °C in air. Seashells were employed as a sustainable CaO source.

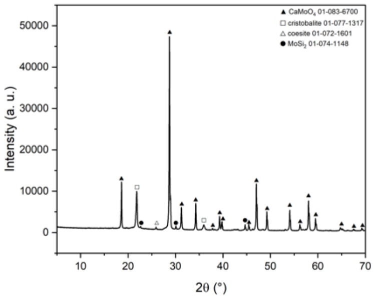

Figure 1. XRD pattern of the sample obtained at 1200°C.

Table 1. Phase composition of the investigated sample obtained at 1200 °C.

	Phase Name	Content (%)
Crystalline (98.13 %)	Calcium Molybdate	56.83
	Cristobalite low, syn	27.58
	Coesite, syn	11.69
	Molybdenum silicide	2.03
Amorphous (1.87 %)		1.87

The obtained precursor mixture was analyzed using thermogravimetric (TG/DTG) methods, revealing that powellite formation occurs at approximately 700 °C. All samples were subsequently annealed in the temperature range of 700–1300 °C. X-ray diffraction (XRD) analysis confirmed that the powellite phase remains stable up to 1200 °C. Additionally, the dielectric properties of the synthesized materials were investigated.

Table 2. Unit cell parameters of the phases identified in the sample obtained at 1200 °C.

	a **(Å)**	***b*** **(Å)**	***c*** **(Å)**
Calcium Molybdate	5.23	5.23	11.43
Cristobalite low, syn	5.00	5.00	6.98
Coesite, syn	7.19	12.42	7.15
Molybdenum silicide	3.20	3.20	7.84

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Isothermal decay analysis of quartz

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The analysis of isothermal decay in thermoluminescence (TL) provides critical insights into the trapping and recombination mechanisms governing luminescence in materials. In first-order kinetics, charge carriers are released from traps without significant retrapping, resulting in a simple exponential decay. However, real-world systems often exhibit deviations from idealized behavior due to competing pathways, retrapping efects, or higher-order kinetics. The linear relationship between ln(I) and time in frst-order kinetics facilitates straightforward determination of activation energy (E), making it a cornerstone of TL analysis. The inclusion of general-order kinetics expands the applicability of these studies by accommodating complex TL behaviors, particularly in fields such as dosimetry and geochronology, where precise trap characterization is vital for accurate dose reconstruction and age determination. By analyzing decay curves at varying temperatures, the resulting slope differences ln(I) versus time plots ofer insights into the underlying kinetic processes.

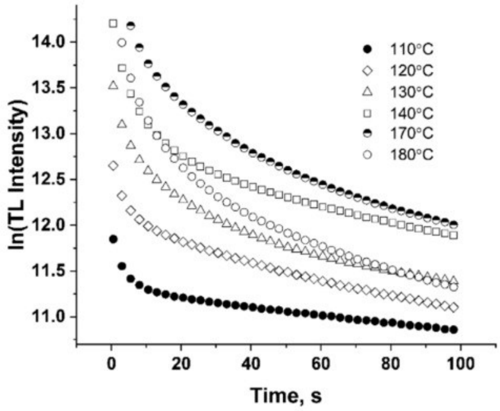


Figure 1. Plot of the natural logarithm of TL intensity versus time at different Tstop temperature. Tstop temperatures are indicated in the legend

Figure 1 illustrates the time-dependent TL intensity decay at constant temperature for quartz samples preheated at 500 °C on a semi-log scale. Subsequently, samples were heated to a predefined Tstop temperature, followed by TL signal recording under isothermal conditions (100 s stabilization). For TL peaks governed by frst-order kinetics, isothermal decay follows an exponential trend, as described in. A linear dependency of ln (TL intensity) versus time plot confrms frst-order behavior, with the slope yielding−E/kT and the intercept corresponding to ln(s/β). Nonlinearity in such plots, however, indicates deviations from frst-order kinetics. The plots generated from the data in Fig. 1 demonstrated nonlinearity, indicating that the TL data does not conform to frst-order kinetics. The general-order kinetics equation suggests that plotting $(I_t / I_0)^{(1-b)/b}$ as a function of time should result in a straight-line relationship when an appropriate kinetic order parameter (b) is selected according to [2]:

$$\left(\frac{I(t)}{I_0}\right)^{\frac{(1-b)}{b}} = 1 + (b-1)\frac{t}{\tau} b \neq 1$$

where I(t) is the intensity of the luminescence signal as a function of time; τ is the lifetime for isothermal decay; and b is the order of kinetics.

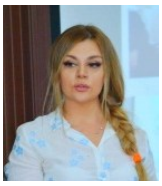
However, when the general-order kinetics approach was applied to the isothermal decay data in Fig. 1 using kinetic order parameters b=1.9,2.0,2.1, and 2.2, none of the tested values produced a statistically valid linear ft. This outcome highlights a fundamental challenge in analyzing isothermal decay data, as subtle graphical variations for different b values complicate the identification of an optimal kinetic order. The persistent lack of linearity across all tested b values strongly suggests that the TL decay does not conform to second-order kinetics. This conclusion was further reinforced by repeating the analysis on additional datasets in Fig. 1, all of which similarly failed to align with second order kinetic behavior.

To explore alternative explanations for the observed decay dynamics, the superposition of two or three exponential functions-each linked to distinct trapping centers-was evaluated [1]:

$$I_t = I_{01} exp\left(-P_1 t\right) + I_{02} exp\left(-P_2 t\right) + \dots$$

where Ion is the phosphorescence intensity due to electrons in the traps of energy En, Pn=s exp (- En/kT) is the probability of an electron escaping from a trap, k is the Boltzmann constant, and s is the escape frequency factor. A detailed decomposition of the decay curves into such components was attempted to resolve individual activation energies (E). However, the results revealed that the decay profiles cannot be accurately modeled as a sum of two or three first-order exponential terms, ruling out a simple superposition of first-order processes.

Subsequent efforts to deconvolute the curves using second order kinetic components also proved unsuccessful, further underscoring the complexity of the underlying trapping-



Ph.D. Aybaniz S. Ahadova is with the Institute of Physics Ministry of Science and Education of the Azerbaijan Republic. Having graduated from Baku State University in 2008, obtained her M.Sc in 2011 and Ph.D. in 2026. Her research interest covers Thermoluminescence and EPR dating of quartz samples.

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recombination mechanisms. Intriguingly, the isothermal decay data were best described by combining two single exponential decay terms with a constant offset, a phenomenon previously reported in studies of natural quartz. For instance, successfully modeled similar isothermal decay profiles using three exponential components and a constant term.

Collectively, the nonlinearity observed in Fig. 1 and analogous datasets in the literature implies that the TL signal arises from contributions of multiple trapping centers. The relative influence of these centers appears temperature dependent, leading to deviations from idealized exponential decay behavior. This complexity challenges conventional kinetic models and underscores the need for advanced analytical frameworks to account for heterogeneous trap distributions and dynamic recombination pathways.

Acknowledgment

The authors thank to the Institute of Archaeology and Antropology for the providing the samples.

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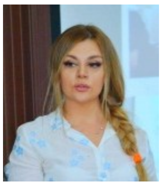

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Investigation of Degradation in Functionalized h-BN/PBI Composite Membranes for HT-PEMFCs

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High-temperature proton exchange membrane fuel cells (HT-PEMFCs) require membranes that maintain proton conductivity, acid retention, dimensional integrity, and chemical stability under hot, low-humidity, and oxidative operating environments [1].

Phosphoric-acid-doped polybenzimidazole (PBI) membranes remain among the most widely investigated HT-PEMFC electrolytes because of their high thermal stability, strong acid–base interaction with H_3PO_4, and suitability for anhydrous proton transport at elevated temperatures, as discussed in comprehensive studies by Li et al. and Escorihuela et al. [1,2]

However, long-term durability is still limited by oxidative degradation, acid leaching, and mechanical weakening, especially when radical species such as •OH and HOO• attack vulnerable sites in the PBI backbone during fuel-cell operation or accelerated Fenton testing [3].

Inorganic filler incorporation has been widely explored to mitigate these limitations by enhancing acid retention, polymer–filler interactions, and membrane resistance against chemical and morphological deterioration. Among these fillers, hexagonal boron nitride (h-BN) is particularly attractive because of its high thermal and chemical stability, electrically insulating character, and layered structure. Hussin, Budak, and Devrim reported PBI/boron nitride composite membranes for HT-PEMFC applications, showing that BN incorporation can improve membrane performance and stability when well dispersed in the PBI matrix [4,5].

Our recently published work on functionalized BN-based PBI composite membranes, including pyridine-PBI/boron nitride systems, demonstrated improved proton conductivity, acid retention, and oxidative resistance through stronger acid–base and hydrogen-bonding interactions among the PBI matrix, phosphoric acid, and functional groups on BN. [5].

In this study, the Fenton-test-induced degradation behavior of functionalized h-BN/PBI composite membranes was investigated for HT-PEMFC applications. After oxidative exposure, the membranes were characterized using FTIR to identify changes in chemical bonding and functional groups, XRD to evaluate changes in amorphous/crystalline structure and h-BN-related diffraction features, and SEM to examine surface morphology, filler dispersion, and degradation-induced defects. Since h-BN-based fillers have been reported to improve the thermal and chemical robustness of PBI composite membranes, this multi-analytical investigation provides insight into how functionalized h-BN contributes to the oxidative durability and structural stability of PBI-based composite membranes for HT-PEMFC operation.

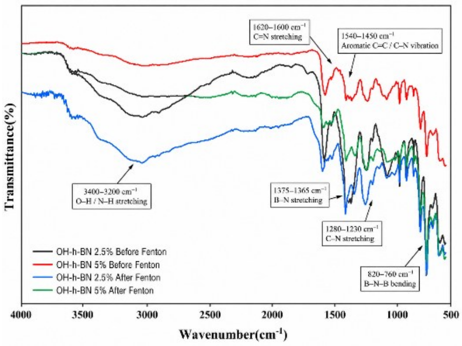

Figure 1. FTIR spectra of P-PBI/OH-h-BN membranes before and after Fenton test.

The FTIR spectra of P-PBI/OH-h-BN composite membranes before and after 8 days of Fenton exposure show the main functional groups of both the P-PBI matrix and OH-functionalized h-BN filler. The broad band at 3400-3200 cm^{-1} corresponds to O-H/N-H stretching, which becomes more pronounced after Fenton treatment, indicating stronger hydrogen bonding and possible oxidation-induced hydroxylated groups. The bands at 1620-1600 cm^{-1} and 1540-1450 cm^{-1} are assigned to C=N stretching of the benzimidazole ring and aromatic C=C/C-N vibrations, respectively [6]. Their changes after Fenton exposure suggest partial oxidative attack on the benzimidazole/aromatic structure. The 1280-1230 cm^{-1} region, related to C-N stretching, also changes after oxidation. The h-BN-related bands at 1375-1365 cm^{-1} and 820-760 cm^{-1}, assigned to B-N stretching and B-N-B bending, remain observable, confirming the stability and reinforcing role of the inorganic filler [5,6].

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Soft-Hard Carbon Synergies for Sodium-ion Battery Anodes

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Sodium-ion batteries benefit from combining hard carbon (HC) and soft carbon (SC) to balance capacity and kinetics. In this work, olive pit derived HC and mesophase pitch derived SC form a synergistic composite anode. The HC+SC electrode delivers higher capacity and better stability than either component alone. This improvement confirms a true synergistic effect beyond simple mixing.

Sodium-ion batteries (NIBs) are widely considered a highly promising and sustainable alternative to lithium-ion batteries for large-scale energy storage applications due to the global abundance and low cost of sodium resources. For NIBs, non-graphitic carbonaceous materials have emerged as the most viable commercial anode candidates. Hard carbon (HC) exhibits a high reversible specific capacity (around 300 mAh/g) and an extended low-voltage plateau (near 0.1 V) driven by a nanopore-filling mechanism, which ensures high overall energy density. However, its highly disordered "house of cards" structure, abundant defects, and large surface area often lead to a low initial Coulombic efficiency (ICE) and sluggish Na^+ diffusion kinetics, which can limit high-power, fast-charging applications.

Conversely, soft carbon (SC) possesses a relatively higher degree of structural ordering, larger carbon layer sizes, and fewer pore structures. The sodium storage mechanism in SC is predominantly governed by interlayer intercalation and surface adsorption rather than pore filling. This provides excellent reversibility, structural stability, and superior rate capability (fast kinetics) in the sloping voltage region. Nevertheless, pure SC lacks an extended low-voltage plateau and can suffer from irreversible capacity loss when Na^+ ions are deeply trapped in certain carbon layers, which restricts its total capacity and energy density.

Integrating these structural motifs into a soft-hard carbon synergistic composite presents an optimal strategy to overcome their individual limitations and achieve high-performance sodium storage. The synergy between the two carbon matrices allows for a meticulously engineered microstructure: the ordered domains of the soft carbon facilitate rapid Na^+ ion transport kinetics and reduce the irreversible consumption of sodium at the solid electrolyte interphase (SEI), while the closed nanopores and expanded turbostratic interlayers of the hard carbon provide ample active sites for quasi-metallic sodium pooling to maximize the plateau capacity. Furthermore, carefully tuning the ratio and defect concentration through this synergistic approach lowers the Na^+ diffusion barriers, preventing the accumulation of "pseudo-dead Na" at the electrode/electrolyte interface and suppressing excessive electrolyte decomposition.

Ultimately, exploiting the soft-hard carbon synergy provides a comprehensive and scalable pathway to design next-generation NIB anodes. By bridging the fast-charging rate performance of soft carbons with the high energy density of hard carbons, this synergistic design promises an optimal balance of high initial Coulombic efficiency, superior power density, and long-term cycling stability [1,2].

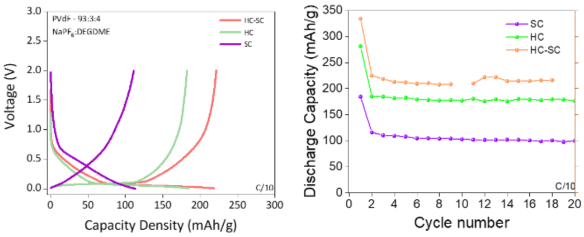

Figure 1. Hard- Soft Carbons electrochemical performances

Here in this work we demonstrate a synergistic interaction between hard carbon (HC) and soft carbon (SC) in the composite anode derived from olive pit–based HC and mesophase pitch–based SC. In the voltage–capacity profiles (Fig. 1), the HC+SC electrode combines the sloping behavior characteristic of SC with the low-voltage plateau associated with HC, indicating the coexistence of different sodium storage mechanisms. More importantly, the composite delivers a significantly higher reversible capacity (~210-220 mAh/g after stabilization) compared to both individual components, exceeding the value expected from their simple linear combination. This enhanced performance, together with its stable cycling behavior, suggests that the mesophase pitch derived SC improves electronic conductivity and reaction kinetics, while the olive pit derived HC provides abundant sodium storage sites, leading to a synergistic effect beyond a mere additive contribution.

Acknowledgements

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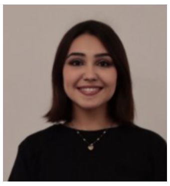

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Linking Phase Stability and Oxygen-Vacancy Energetics in High-Entropy Oxide Nanofibers via Machine-Learned Potentials

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High-entropy oxide (HEO) nanofibers are promising architectures for electrochemical energy storage electrodes. They combine high surface area, compositional tunability, and multi-cation redox activity. However, the same compositional flexibility that enables property optimization makes it difficult to identify single-phase stability windows and oxygen vacancy energetics across dopant space using density functional theory (DFT) alone. Here, we integrate electrospun HEO nanofiber experiments with universal machine learned interatomic potential (uMLIP/UMA) modeling and stability descriptors to connect synthesis outcomes with composition–stability predictions.

Experimentally, Mn- and Ti-doped equiatomic (CoCuMgNiZnX)O nanofibers (X = Mn, Ti) preserve a continuous, interconnected network after calcination, exhibiting mild crystallization-induced surface roughness and high BET surface areas. XRD verifies a single phase fcc rocksalt structure for Mn-doped fibers, whereas achieving a fully single-phase rocksalt state in Ti-doped fibers using Ti addition alone remains challenging, consistent with a narrower stability margin.

Computationally, we employ uMLIP/UMA (CHGNet and eSEN) to map single-phase stability regions using descriptors based on mixing enthalpy and first-nearest-neighbor bond-length disorder [1].

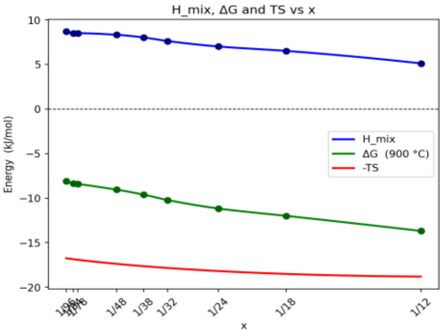

Figure 1. Impact of concentration of titanium (x) in HEO to Gibbs free energy

In the MgCoNiCuZn-Mn compositional space, the model predicts a stable single-phase region at low Mn contents that transitions to multiphase behavior as Mn increases. In contrast, coupled Ti-Li substitution enhances thermodynamic stability, with configurational entropy contributions becoming increasingly important in lowering Gibbs free energy at elevated temperatures (≈900 °C). uMLIP defect calculations further reveal strong cation control of oxygen vacancy formation energies. [2] Overall, this combined experimental-computational framework positions uMLIP as a practical route to predict phase boundaries and vacancy stability and to interpret experimentally observed single- versus mixed-phase outcomes in doped rocksalt HEO nanofibers.

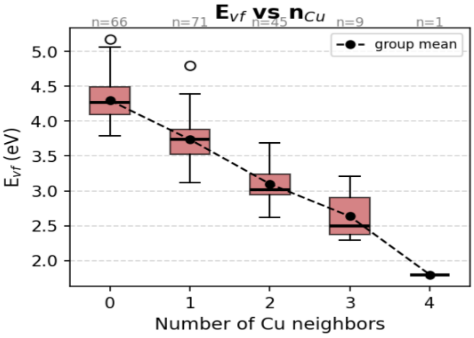

Figure 2. Vacancy formation energy dependence on copper content

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Electrochemical Noise Analysis Coupled with EIS Interpretation in Li/MnO_2 Primary Batteries

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Primary lithium batteries continue to serve as a dominant energy source for a wide range of commercial applications; however, their performance can deteriorate in an unpredictable manner under abusive conditions such as external short circuits or prolonged self-discharge. The initial degradation processes primarily originate at the anode interface, where localized lithium depletion leads to changes in reaction kinetics and disrupts interfacial uniformity. Conventional diagnostic techniques typically identify these effects only after significant damage has occurred, underscoring the need for minimally invasive, highly sensitive methods capable of tracking interfacial evolution in real time.

In earlier work, we demonstrated that Li/MnO_2 cells show a marked increase in electrochemical noise under short-circuit conditions, suggesting that noise characteristics are strongly influenced by interfacial states. [1] Nevertheless, the underlying mechanisms and their relationship to electrochemical reaction pathways remained insufficiently understood, motivating a more integrated and correlative investigation. In this study, CR2032 Li/MnO_2 cells were subjected to short-circuiting for periods of up to three days, during which electrochemical impedance measurements were conducted under small-signal perturbations. Simultaneously, higher-order harmonic components and noise amplitudes were analyzed to probe nonlinear interfacial behavior. These electrochemical findings were further correlated with surface imaging of the anode to confirm the development of heterogeneity.

As lithium depletion becomes non-uniform, an increase in charge-transfer resistance is observed alongside the emergence of odd harmonics, indicating the onset of interfacial asymmetry. With continued depletion, even harmonics and overall noise levels rise, reflecting the presence of multiple concurrent reaction pathways. By the second day, the third harmonic reaches its maximum intensity, corresponding to a highly heterogeneous interface characterized by the coexistence of lithium clusters and exposed stainless-steel regions. When lithium is nearly exhausted by the third day, harmonic intensities diminish toward the baseline despite elevated impedance values, suggesting a transition to reaction mechanisms dominated by the metallic substrate.

This study explores the combined use of electrochemical impedance spectroscopy and harmonic noise analysis as a means to improve early detection of degradation in Li/MnO_2 primary batteries. The objective is to establish a mechanistic connection between impedance changes, nonlinear interfacial dynamics, and spontaneous voltage fluctuations associated with lithium depletion processes.

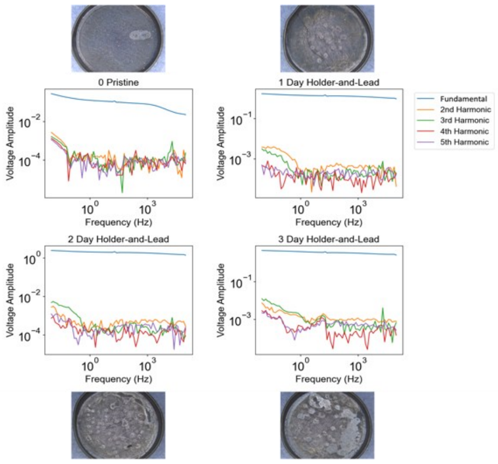

Figure 1. Harmonic spectra and corresponding anode images of CR2032 coin cells are presented shorted through for 1, 2 and 3 Days and a pristine cell.

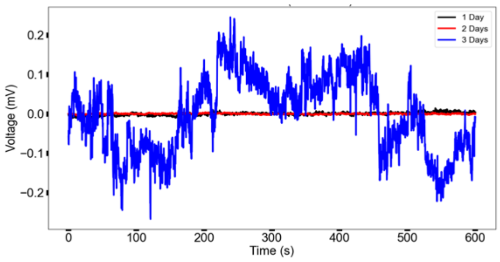

Figure 2 Electrochemical voltage noise for Li/MnO_2 CR2032 coin cells and lithium anode images for shorted cells after 1, 2, and 3 days (black, red, blue)

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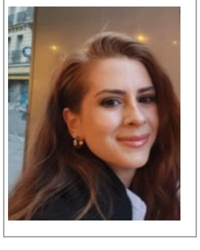

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From vast MXene design space to synthesizable MXENE/PANI composites: embedding guided, model driven interface engineering

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Conductive polymers such as polyaniline (PANI) are attractive building blocks for hybrid functional materials, but their macroscopic performance often hinges on poorly understood polymer–surface interactions and the immense combinatorial space of compatible inorganic hosts.

Here, we present a multimodal, data driven strategy to discover and rationally design MXene/PANI hybrids across a broad range of applications including aqueous/ambient energy materials, sensing, and flexible electronics. We systematically explore a vast mixed composition MXene design space using existing databases [1] and descriptors for MXene stability [2]. In search we impose practical constraints on stability, termination chemistry and electronic transport potential.

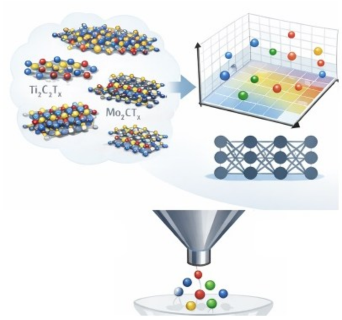

Figure 1. Exploring compositional variations on MXene side by combining elemental embeddings and stability screening

To enrich chemical representations beyond conventional elemental descriptors, we integrate literature derived static word embeddings as elemental features [3] and use them as composition-property predictors.

Interactions between ES PANI and selected MXene surfaces are assessed using universal atomistic UMA models to rapidly identify stable interfaces and binding motifs.

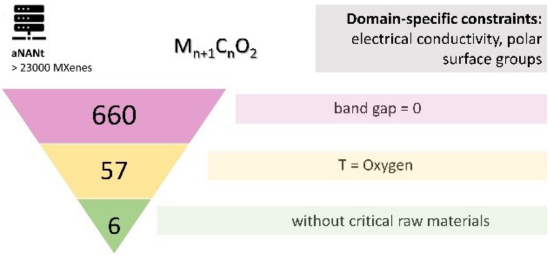

Figure 2. Selecting suitable MXene materials from aNANt database

Finally, we synthesize and characterize Ti_2CT_x/ES-PANI composites to validate predicted interaction trends and extract experimentally grounded design rules linking MXene chemistry and interfacial stability.

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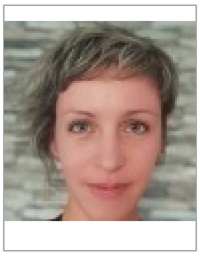

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Design of Composite SOFC Cathodes via Spray Pyrolysis: Synergistic Effects of Perovskite and Ruddlesden–Popper Phases

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Intermediate-temperature solid oxide fuel cells (IT-SOFCs, 600–800 °C) have attracted considerable attention due to their potential for high efficiency and reduced operating costs. However, the sluggish oxygen reduction reaction (ORR) kinetics at lower temperatures remains a key limitation, making the development of high-performance cathode materials essential.

Perovskite-type oxides such as LSC113 exhibit high electronic conductivity and excellent catalytic activity, whereas Ruddlesden–Popper (RP) phases like LSC214 provide enhanced oxygen ion transport and improved structural stability. The combination of these two structures is expected to synergistically enhance both surface oxygen exchange and bulk diffusion processes. In addition, Fe-containing counterparts (LSCF-based systems) offer improved thermal stability and better compatibility with electrolyte materials.

In this study, composite cathodes based on LSC and LSCF based systems were synthesized using a solution-assisted deposition approach that enables the formation of homogeneous and porous microstructures. The electrochemical performance of the prepared cathodes was evaluated through area-specific resistance (ASR) measurements to assess their ORR activity and identify compositions with improved performance for intermediate-temperature SOFC applications.

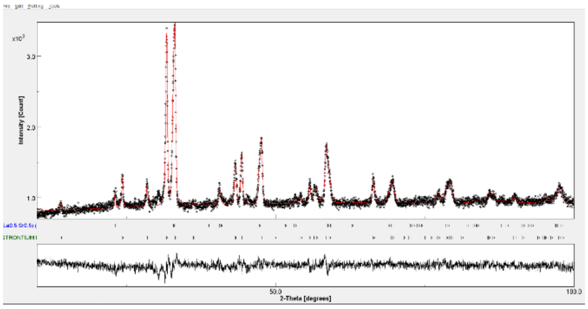

Figure 1. XRD plot of LSC113 and LSC214 cathode material coated on GDC by Ultrasonic Spray Pyrolysis.

The precursor solution used for the coating process was prepared using a solution-based approach involving metal salts dissolved in a mixed solvent system. The synthesis parameters were adjusted to obtain a stable solution suitable for controlled deposition, and further optimization was carried out based on experimental observations.

X-ray diffraction analysis (Figure 1) revealed that the synthesized sample predominantly consists of an RP-type phase, accompanied by a minor perovskite contribution. This indicates that the selected synthesis conditions favor the formation of the RP structure while allowing partial coexistence of both phases. The refinement results demonstrated good agreement between experimental and calculated patterns, confirming the reliability of the phase identification and structural analysis.

A solution-based deposition technique (Figure 2) was employed for the fabrication of SOFC cathodes, offering several advantages over conventional methods. One of its key benefits is the ability to produce homogeneous and compositionally controlled films, which is particularly important for multi-component oxide systems such as LSC and LSCF. The process enables the formation of fine and uniform microstructures with high surface area and tailored porosity, which are essential for enhancing oxygen reduction reaction (ORR) kinetics.

In addition, the employed approach provides a scalable and cost-effective route for coating on various substrates, including complex geometries. It also allows flexible control over processing conditions, facilitating the optimization of cathode performance. Furthermore, the direct formation of oxide phases during deposition minimizes the need for extensive post-treatment steps, making this technique a promising strategy for the development of efficient and high-performance SOFC cathodes.

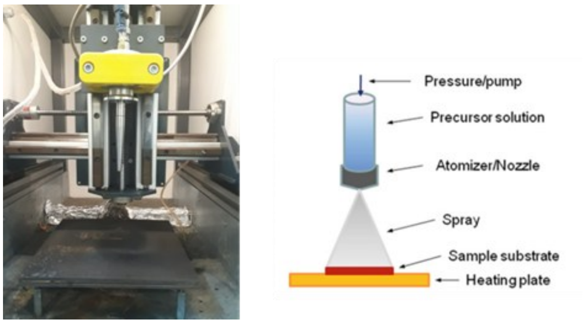

Figure 2. Ultrasonic Spray Pyrolysis.

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Practical High Energy Na-Ion Batteries with Sn-Based Composite Anodes

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Currently, sodium-ion batteries (SIBs) are emerging as the most promising alternative to lithium-ion batteries (LIBs) for large-scale energy storage applications, driven by the natural abundance of sodium, its low cost, and its electrochemical properties being comparable to those of lithium. However, the large ionic radius of sodium (Na^+) limits its insertion into graphite, the traditional anode material for LIBs. Therefore, the success of SIB technology depends significantly on the development of suitable anode materials. Hard carbon, with its large interlayer spacing and irregular microstructure, is considered one of the most viable anode materials for SIBs. The selection of the precursor material for hard carbon synthesis is critical for both cost-effectiveness and electrochemical performance. Due to its high carbon content, abundant availability, and economic viability, coal is viewed as a highly attractive and sustainable precursor for industrial-scale hard carbon production [1].

To enhance the inherently limited capacity of hard carbon materials, incorporating tin (Sn) which offers a high theoretical capacity of 847 mAh/g is a highly effective strategy [2]. Nevertheless, Sn anodes experience severe volume expansion during charge/discharge cycles, leading to loss of structural integrity and rapid capacity decay. This study aims to overcome these challenges by developing a Sn-based composite anode.

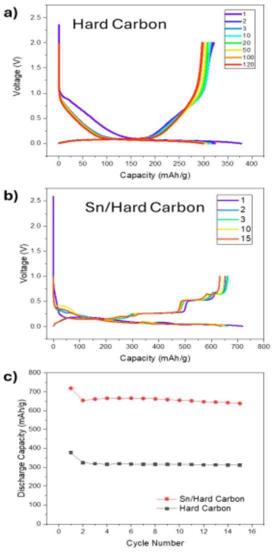

Figure 1. Galvanostatic charge-discharge profiles a) hard carbon, b) Sn/hard carbon and c) Cycling performances for hard carbon and Sn/hard carbon.

According to the results shown in Figure 1, the hard carbon anode synthesized at 1250 °C exhibited a capacity of 299 mAh/g after 120 cycles, with about 92% capacity retention at a current density of 30 mA/g. Preliminary results from the Sn/hard carbon composite anode indicate that the material achieved a capacity of 638 mAh/g, demonstrating stable performance at a current density of 50 mA/g after 15 cycles. Hard carbon derived from coal prevented structural degradation by buffering the severe volumetric expansion of tin particles during sodium insertion. As a result, Sn/hard carbon composites present an ideal anode for next-generation sodium-ion batteries, offering low cost, high capacity, and long cycle life.

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MgH_2 morphological and structural changes during high-energy ball milling

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The dynamic development of the hydrogen economy creates a real alternative to conventional energy carriers. One barrier to widespread implementation worldwide is the lack of a cheap, effective, and safe method of hydrogen storage. Hydrides are a promising method for storing hydrogen, and this approach has been rapidly developing in recent decades [1]. One of the most popular metal hydrides for numerous research groups is magnesium hydride (MgH_2). Magnesium hydride is characterized by a relatively high hydrogen capacity of 7.6 wt.% H_2, high availability and relatively low cost of production. The magnesium hydride decomposition reaction is a fully reversible reaction [2]. Unfortunately, magnesium hydride has two major limitations. namely, the high desorption temperature of 325-425°C and relatively slow hydrogen release kinetics.

The most commonly used methods of hydride destabilization involve lowering the decomposition temperature, such as mechanical milling, which results in a nanostructurization of MgH_2 powder and a reduction in particle size [3].

The study examines the impact of milling time (10s to 5 h) on the structural properties of MgH_2. It reveals a direct correlation between reduced crystallite/particle sizes and decreases in both the decomposition temperature and the activation energy. The results highlight how mechanical milling optimizes hydrogen release kinetics by tailoring the material's microstructural parameters.

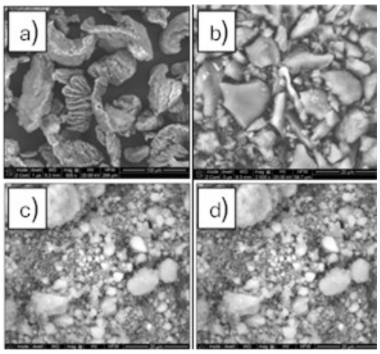

Figure 1. The morphology of the MgH_2 powders: as-received (a) and after milling for 10 s (b), 15 min (c), and 300 min (d).

The morphology of the as-received and milled magnesium hydride powders, presented in Fig. 1, was characterized by the presence of flake-like and irregular globular particles, respectively. It should be noted that a clear reduction in the particle size of the powder and a change from flake-like to globular shapes were observed after only 10 s of milling. Additional morphological changes were essentially reduced to a nonsignificant reduction in the average particle diameter and an increase in the amount of finely crushed particles. Changes in the morphological parameters of the powders are presented in Table 1.

Table 1. Morphological properties of the MgH_2 powder before and after milling for various times.

Properties	**Milling time**			
	0 s	**10 s**	**15 min**	**300 min**
Diameter[1] [μm]	28.0±12.8	10.1±9.6	9.5±8.8	9.3±5.8
Diameter[2] [μm	4.42	0.50	0.33	0.39

[1]Average Dn diameter measured by IPS. [2]Diameter measured using the BET technique

For the material in polycrystalline and submicrometric forms (up to 300 nm), we observe a slight decrease in the decomposition temperature, reflecting a decrease in the activation energy. This step is typical of mechanical activation and is associated with an increase in the fraction of chemically active powder particles' fresh surfaces. With a decrease in crystallite size to the nanoscale (100 nm), we observe a linear relationship between crystallite size and decomposition temperature, as reported in numerous studies on the influence of nanostructuring processes on the sorption properties of MgH_2.

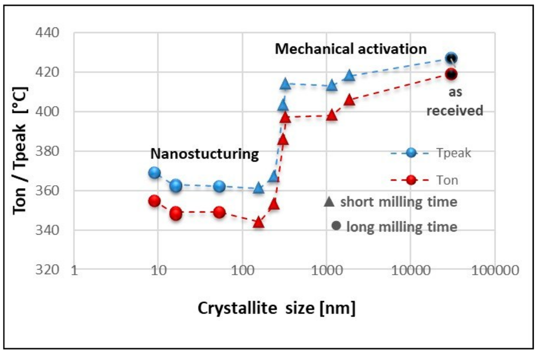

Figure 2. The changes in decomposition temperature for MgH_2 vs. crystallite size [3].

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Development of hydrogen compressors

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1. Introduction

As the world shifts toward a decarbonized energy landscape, hydrogen has emerged as a critical vector for clean energy storage and transport. However, because of hydrogen's extremely low volumetric density, efficient and reliable compression is essential for its practical deployment. The thermal driven (TD) hydrogen compression is the technique with its advantages (no moving parts, potentially better reliability and endurance) but also drawbacks, such as low efficiency and external heat dependence, which can be compensated with industrial waste heat [1][2].

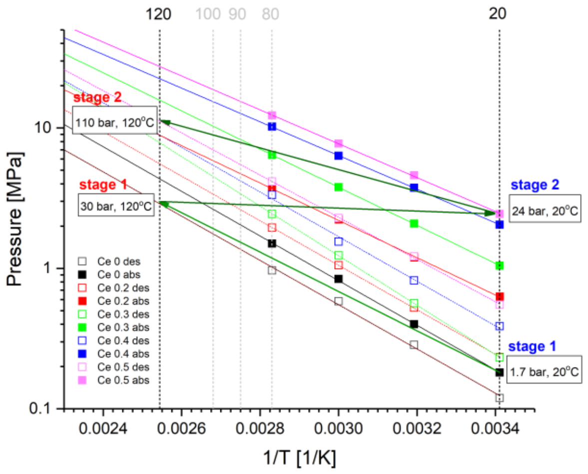

Figure 1. Possible hydrogen sorption path for two stage thermal driven compressor with Ce doped AB5 active material.

We are committed to development of hybrid system with hydrogen storage plus two stage thermal driven compression system with output pressure up to 110 bars. The compression stage is based on AB5 active material. The storage stage is metal hydride based with desorption pressure sufficient to drive stage 1 with initial pressure of 1.7 bar as 20°C. By subsequent heating of the stage 1, transferring hydrogen to low temperature stage 2 and heating of the stage 2, output pressure is set desired value. A half cycle system has been constructed, meaning the hydrogen supply is possible only when the stage 2 is in heating stage. In the prospect we are planning the development of full cycle system with additional two "mirror" stages operating in opposite heating/cooling phases, thus enabling the continual supply of hydrogen.

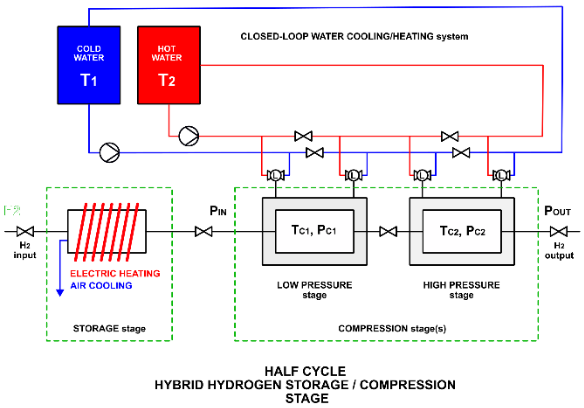

Figure 2. Block diagram of half-phase hybrid hydrogen storage/compression system.

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Dr. Jasmina Grbović Novaković has made significant contributions to the 'Vinča' Institute and the Republic of Serbia through her research in hydrogen energy materials, playing a key role in laying the foundation for the nation's energy transition. Through the establishment of the Center of Excellence (CONVINCE) and a joint Chinese-Serbian laboratory, she enhanced the Institute's research capabilities, positioning it as a regional center for renewable energy. Her professional portfolio highlights her participation in drafting Serbia's Hydrogen Energy Development Strategy and Montenegro's Green Hydrogen Strategy project.

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Comparative Electrochemical Performance Analysis of NMC Cathodes Obtained from Recovered and Commercial Materials

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The increasing demand for lithium-ion batteries has intensified interest in sustainable material sourcing; however, the electrochemical validation of regenerated cathode materials remains insufficient [1]. While numerous studies focus on material recovery processes, the extent to which regenerated cathodes can match the electrochemical performance of their commercial counterparts is still not fully established [2].

In this study, cathode active material was mechanically separated from end-of-life lithium-ion batteries and subsequently regenerated via a green hydrometallurgical process. By optimizing the recovery conditions, the compositional properties of the regenerated cathode material were carefully tuned. The recovered material was then re-synthesized and reused in the fabrication of new lithium-ion battery cells. The electrochemical performance of the recovered $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (R-NMC) cathode was systematically evaluated and directly compared with that of a pristine, commercially available NMC material. This approach enables a comprehensive assessment of the functional performance of the regenerated cathode under identical conditions, providing insight into its practical applicability in new battery systems.

Figure 1. Cathode electrode coated via slurry-casting method.

In current research, recovered cathode active material was used to prepare working electrodes via a conventional slurry-casting method (Figure 1). The electrode composition consisted of 75 wt% active material, 15 wt% conductive carbon (Super P), and 10 wt% poly(vinylidene fluoride) (PVDF) binder dispersed in N-methyl-2-pyrrolidone (NMP). The homogeneous slurry was coated onto carbon-coated aluminum foil and subsequently dried under vacuum at 100 °C overnight. For comparison, a commercial $LiNiMnCoO_2$ (C-NMC) cathode powder (Sigma Aldrich) was processed under identical conditions to fabricate reference electrodes. CR2032-type coin cells were assembled using lithium metal as the counter/reference electrode, a polypropylene separator, and 1 M $LiPF_6$ dissolved in ethylene carbonate/dimethyl carbonate (1:1 vol) as the electrolyte. After assembly, the cells were rested at open-circuit voltage for 12 h prior to testing. Charge and discharge tests were carried out in the voltage range of 2.7-4.3 V on Gamry Reference 3000 Potentiostat/Galvanostat/ZRA at various current densities (1C = 170 mA g^{-1}) at 25ºC. Electrochemical impedance spectroscopy (EIS) measurements were conducted over a frequency range of 0.01 Hz to 10 kHz with an AC amplitude of 5 mV.

Table 1. Electrochemical parameters of recovered and commercial NMC cathode powder. (0.1C)

	Initial Discharge Capacity (mAh.g^{-1})	**Initial Columbic Efficiency (%)**
R-NMC	158.8	92
C-NMC	162.4	96

Electrochemical results show that the recovered NMC maintains a competitive and stable performance with good reversibility and strong rate capability compared to commercial NMC (Table 1). The high- to mid-frequency semicircle in the Nyquist plot corresponds to the combined effects of surface film resistance (R_F) and charge transfer resistance (R_{CT}) at the electrode–electrolyte interface. In the low-frequency domain, the sloped linear response is characteristic of Warburg impedance (Zw), reflecting the diffusion behavior of lithium ions within the system. The R_{CT} values of the synthesized NMC and the commercial counterpart were found to be quite comparable. This indicates that the recovered material exhibits electrochemical behavior similar to that of the commercial sample. These findings are in good agreement with the XRD and SEM-EDS results, confirming that the regenerated material preserves its layered structure and compositional homogeneity.

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Illumination-Dependent Electrochemical Impedance Analysis of Bi_2O_3-Based photoelectrodes

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Bismuth oxide (Bi_2O_3) has attracted considerable attention as a multifunctional material for electrochemical energy storage and optoelectronic applications due to its favorable redox activity, semiconducting properties, and tunable morphology [1]. Despite these advances, the influence of substrate, interfacial properties, and external factors such as applied potential and illumination on the electrochemical behavior of Bi_2O_3 thin films remains insufficiently explored. This paper presents the results of EIS analysis of Bi_2O_3-based thin films.

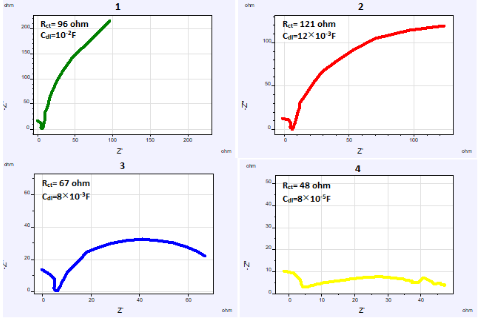

Figure 1. Nyquist impedance spectra for the Ni/Bi_2O_3 electrode in 0.5 M Na_2SO_4 solution at various potentials. (1) −0.4 V (2) −1.15 V; (3) −1.25 V; (4) −1.5 V.

The electrochemical impedance spectroscopy (EIS) results of the Ni/Bi_2O_3 electrode in 0.5 M Na_2SO_4 at different applied potentials are presented as Nyquist plots in Fig. 1. Each spectrum exhibits a depressed semicircle in the high-to-medium frequency region followed by a low-frequency tail, indicating the coexistence of charge transfer and diffusion-controlled processes. The diameter of the semicircle, corresponding to the charge transfer resistance (Rct), shows a strong dependence on the applied potential. At **−0.4 V,** a relatively large semicircle (Rct ≈ 96 Ω) is observed, suggesting sluggish electron transfer kinetics and limited electrochemical activity. As the potential shifts to −1.15 V, the Rct increases further (≈121 Ω), which may be attributed to the adsorption of reaction intermediates or partial blockage of active sites on the electrode surface. Upon increasing the cathodic potential to −1.25 V, the Rct decreases significantly (≈67 Ω), indicating enhanced charge transfer and improved reaction kinetics. At −1.5 V, the smallest semicircle is obtained (Rct ≈ 48 Ω), reflecting highly facilitated electron transfer and increased electrocatalytic activity. Additionally, the more pronounced low-frequency tail at higher overpotentials suggests that diffusion processes become dominant. Overall, these results demonstrate that increasing the cathodic potential activates the electrode surface and promotes faster electrochemical reactions, likely associated with reduction processes such as hydrogen evolution.

The decrease in Rct with increasing negative potential confirms the enhanced electrocatalytic activity of the Ni/Bi_2O_3 electrode.

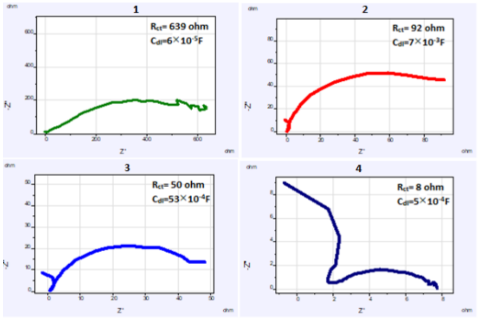

Figure 2. Nyquist impedance spectra for the Ni/Bi2O3 electrode in 0.5 M Na2SO4 solution at various potentials were carried out under illumination. (1) −0.4 V (2) −1.15 V; (3) −1.25 V; (4) −1.35 V.

The corresponding charge (Rct) and double-layer capacitance (Cdl) values were obtained by fitting the experimental data using an equivalent circuit model. A significant decrease in R_ct is observed with increasing cathodic potential, indicating enhanced charge transfer kinetics at more negative potentials. Specifically, Rct decreases from 639 Ω at −0.40 V to 8 Ω at −1.35 V, suggesting improved electrochemical activity of the Ni/Bi_2O_3 electrode under illumination. Meanwhile, the variation in Cdl reflects changes in the electrochemically active surface area and interfacial properties.

The combined effect of illumination and applied potential significantly enhances the interfacial charge transfer kinetics, highlighting the potential of the Ni/Bi_2O_3 system for photoelectrochemical applications.

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Tailoring Surface Chemistry of Ni and Co overlayers on $BiVO_4$ Thin Films for enhanced solar fuel production

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Bismuth vanadate ($BiVO_4$, BVO) is widely recognized as one of the most promising photoanode materials for photoelectrochemical (PEC) fuel production due to its suitable bandgap, efficient visible light absorption, and thermodynamic stability over a wide potential–pH range. However, its performance is fundamentally limited by sluggish surface reaction kinetics and significant charge recombination losses. To address these challenges, cocatalyst engineering has emerged as an effective strategy to enhance interfacial charge transfer and accelerate kinetics of solar fuel production.

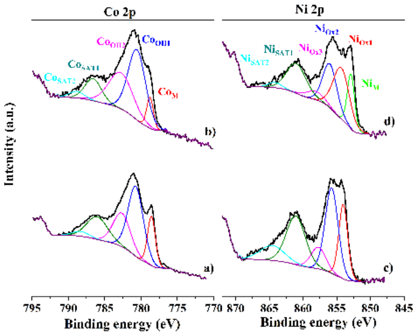

Figure 1. Co 2p and Ni 2p XPS spectra of a) BVO_Co, b) BVO_Ni_Co, c) BVO_Ni and d) BVO_Co_Ni

In this work, we systematically investigated the impact of ~3 nm Ni and Co layers, deposited via sputtering, on the physicochemical properties and oxygen evolution reaction (OER) efficiency of hydrothermally synthesized BVO thin films. The samples are denoted as BVO (pristine), BVO_Ni and BVO_Co (single cocatalysts), and BVO_Ni_Co and BVO_Co_Ni for sequentially deposited bilayers.

The impact of the engineered surface chemistry is reflected in the linear sweep voltammetry results, where the BVO_Ni_Co sample exhibits the highest photocurrent density, delivering an approximately six-fold increase in photocurrent at 1.23 V vs RHE compared to pristine BVO and clearly outperforming all other configurations. This trend is further supported by IPCE measurements indicating more efficient photogenerated charge utilization. A more detailed analysis of charge transport processes (**Table 1**) reveals that pristine BVO exhibits low bulk and surface charge transport efficiencies, resulting in negligible overall performance. Upon cocatalyst deposition, distinct functional roles emerge: Co predominantly enhances bulk charge separation, while Ni improves surface charge transfer, leading to a substantial increase in ABPE compared to pristine BVO. Notably, the sequence of deposition plays a decisive role, with the Ni→Co configuration delivering the highest bulk efficiency (η_T = 38%) and overall performance (ABPE = 0.14%). These findings underscore that optimal PEC performance is governed by a delicate balance between bulk charge transport and surface reaction kinetics.

Table 1. Charge transport efficiencies in the bulk (**η_T**) and at the surface (**η_I**) of BVO and maximal applied-bias photocurrent efficiency (ABPE).

Sample	η_T (%)	η_I (%)	ABPE (%)
BVO	9	15	0.014
BVO_Co	29	21	0.09
BVO_Ni	17	31	0.09
BVO_Co_Ni	14	36	0.07
BVO_Ni_Co	38	20	0.14

XPS analysis (**Figure 1**) confirms the presence of Ni and Co species on the BVO surface, revealing mixed oxidation states characteristic of catalytically active oxide and oxyhydroxide phases. Furthermore, depth-resolved XPS measurements reveal a non-uniform distribution of cocatalysts. In particular, Co remains predominantly in hydroxide-like form at the surface, acting as the primary catalytic site for OER, while Ni exhibits a depth-dependent distribution, transitioning from a thin oxidized layer (NiO) at the surface to a subsurface metallic Ni^0 region. This metallic Ni acts as an efficient charge-transfer medium, facilitating electron transport from the BVO bulk toward the surface catalytic sites. The resulting vertical chemical gradient enables strong electronic coupling, reduced charge-transfer resistance, and improved charge separation, ultimately leading to the superior PEC performance of the BVO_Ni_Co photoanode.

Overall, this work demonstrates that the performance of BVO photoanodes is governed not only by cocatalyst composition but critically by their spatial distribution and interfacial electronic structure. This study establishes architectural engineering of cocatalysts as a strategy for advancing high-efficiency PEC systems.

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Sustainable Rare Earth Recovery Using Nicotinium-based Ionic Liquid Polymer Inclusion Membranes

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Rare earth elements (REEs), particularly neodymium (Nd), are indispensable raw materials widely used in advanced energy storage technologies and various electronic devices. The increasing accumulation of battery and electronic waste has intensified the need for sustainable and selective method for recovery and recycling of rare earth elements. One promising approach involves the use of polymer inclusion membranes (PIMs) combined with ionic liquids (PIM-ILs). This technique has attracted considerable attention due to its low solvent consumption, simple preparation procedure, and environmental benefits.

In this study, a homologous series of nicotinium-based ionic liquids with different alkyl chain lengths was synthesized. Subsequently, PIM-ILs containing the synthetized ILs were prepared and characterized, and finally, applied for Nd (III) extraction. The synthesized ILs included N-octylnicotinium bromide (C8NicBr), N-decylnicotinium bromide (C10NicBr), N-dodecylnicotinium bromide (C12NicBr), and N-tetradecylnicotinium bromide (C14NicBr). The variation in alkyl chain length was introduced to investigate its influence on membrane performance, membrane stability and extraction efficiency. Structural characterization and confirmation of successful synthesis were performed using Fourier-transform infrared spectroscopy (FTIR).

Membrane fabrication involved dissolving poly(vinyl chloride) (PVC) and the IL in an 80 : 20 ratio in tetrahydrofuran (THF). The resulting homogeneous solutions were cast onto glass Petri dishes and left to stand at ambient temperature overnight to allow gradual solvent evaporation. After complete solvent removal, the membranes were carefully detached from the substrate and employed without further modification (Fig. 1).

Figure 1. Nicotinium-based polymer inclusion membranes (PIMs) synthetized in this study.

The extraction efficiency of Nd(III) was assessed under acidic conditions using a laboratory-scale membrane system equipped with distinct feed and stripping aqueous phases (Fig. 2).

Figure 2. Laboratory extraction system based on PIM.

The obtained results showed an Nd(III) recovery of approximately 60% after 30 h. The findings demonstrated effective transport of neodymium across the prepared membranes, thereby confirming the potential of nicotinium-based ionic liquids as selective carriers for rare earth element extraction. Furthermore, the alkyl chain length of the ionic liquids was found to influence membrane performance, with longer alkyl chains contributing to improved extraction efficiency and membrane stability. The experimental configuration enabled a systematic evaluation of Nd(III) transport through the prepared PIM-ILs, allowing the influence of ionic liquid structure on extraction performance to be assessed and demonstrating the potential of these membranes for selective rare earth element recovery from acidic aqueous solutions.

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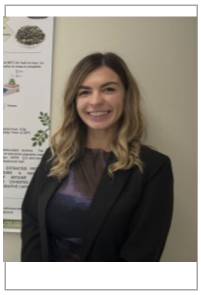
This work was supported by the FREECOVER project — *"Advancing Eco-Friendly Hydrometallurgy for Sustainable Rare Earth Element Recycling and Circular Economy Innovation"*. The project has received funding from the European Union's Horizon Europe research and innovation programme under Grant Agreement No. 101158453.



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Polymorphism and Transition Metal Doping in $NaFeO_2$-Based Cathodes

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Lithium-ion batteries currently dominate the rechargeable battery market; however, safety concerns, the uneven distribution of their constituent elements (Li, Co, and Ni), and their negative environmental impact necessitate the exploration of alternative technologies. Sodium-ion batteries (SIBs) are considered a promising alternative to lithium-ion batteries because they operate on similar principles and benefit from the abundant and sustainable availability of sodium resources [1]. Commercial SIBs commonly employ layered oxide cathodes containing Co and Ni, whose use should be minimized due to their uneven distribution and adverse environmental impact [2].

This study focuses on the synthesis of potential cathode materials composed of earth-abundant and environmentally benign elements. The novelty of our research lies in the use of Fe_3O_4 as the iron precursor, synthesized via precipitation from an aqueous solution of $FeSO_4$ and NaOH. In addition to $FeSO_4$ being significantly less expensive than Fe_2O_3, the use of Fe_3O_4 synthesized from $FeSO_4$ facilitates easier cationic doping of the parent structure. Aqueous solutions of $CuSO_4$ and $MnSO_4$ were added during the precipitation process in cases where doped compounds were synthesized. Solid-state reactions were carried out in a chamber furnace in air at temperatures ranging from 600 to 1000 °C.

It was found that the formation of either the α-$NaFeO_2$ or β-$NaFeO_2$ polymorph is influenced by both the choice of sodium precursor and the calcination temperature due to the topotactic nature of the reaction. The obtained $NaFeO_2$ polymorphs exhibit hygroscopic behavior, requiring additional precautions during the assembly of electrochemical cells. For this reason, attempts were made to synthesize materials with improved moisture resistance. Our approach involves modifying the structure through isomorphous transition-ion substitution, with nominal compositions $NaFe_{0.5}Mn_{0.5}O_2$ and $Na_{0.9}Cu_{0.2}Fe_{0.3}Mn_{0.5}O_2$.

Table 1. Lattice parameters

Lattice parameters [Å]	*a*	*b*	*c*
$NaFe_{0.5}Mn_{0.5}O_2$	2.95574	2.95574	16.45573
$Na_{0.9}Cu_{0.2}Fe_{0.3}Mn_{0.5}O_2$	2.92960	2.92960	11.24366

The crystal structures were refined using the Rietveld method implemented in Topas software [3]. Lattice parameters are given in Table 1. There is significant difference of interlayer spacing along the c-axis which is important for sodium-ion diffusion. Structural analysis revealed that these compounds crystallize in layered structures belonging to the $P6_3/mmc$ and R-3m space groups, respectively (Figure 1). In both structures, oxygen atoms form close-packed layers, while sodium and transition-metal ions occupy alternating interlayer sites. Transition metal T_MO_6 edge-sharing octahedra form $(FeO_2)n$ sheets, between which sodium ions are inserted with an octahedral or prismatic environment. These structures are similar to the structure of α-$NaFeO_2$ polymorph.

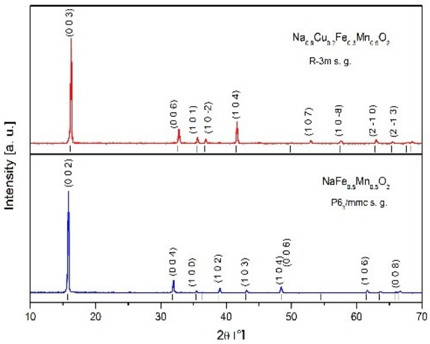

Figure 1. The XRD patterns of manganese and copper doped $NaFeO_2$.

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Electrochemical Noise as a Direct Probe for Copper Deposition Uniformity

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Electrochemical noise (EN) measurements have long been used to study stochastic electrochemical behavior, particularly in corrosion science [1]. Their use in battery research, however, is still emerging [2]. In rechargeable battery systems, especially lithium-based systems, non-uniform electrodeposition can cause dendritic growth, short circuits, and capacity loss [3]. Optical techniques provide valuable information about deposition morphology, but they are not practical for operando studies in sealed commercial cells. EN offers a complementary, non-invasive and non-perturbing route for probing interfacial changes through naturally occurring potential fluctuations.

In this work, copper electrodeposition is used as a controlled model system to evaluate EN as a diagnostic tool for deposition uniformity. Copper is particularly suitable because its deposition behavior is well established, its morphology can be tuned by changing deposition conditions, and the resulting surface features can be directly compared with optical observations [4]. Copper surfaces were first prepared under different deposition conditions to obtain relatively uniform and intentionally non-uniform morphologies. After surface preparation, voltage noise was measured under open-circuit conditions, allowing the effect of morphology on potential fluctuations to be evaluated without applying an additional perturbation during the noise measurement.

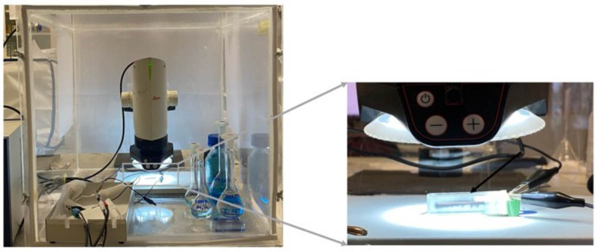

Figure 1. Experimental setup used for in situ optical monitoring during electrochemical noise measurements. The electrochemical cell was placed inside a transparent enclosure and monitored using a digital microscope positioned above the quartz cuvette. The magnified image shows the cuvette region where copper electrodes were observed during deposition and subsequent voltage noise measurements.

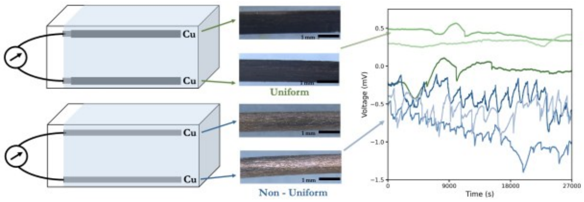

Figure 2. Correlation between copper surface morphology and voltage noise response. Representative optical images of uniformly and non-uniformly deposited copper surfaces are shown together with their corresponding open-circuit voltage noise signals. Uniform copper surfaces exhibit lower-amplitude fluctuations, whereas non-uniform surfaces show larger and more irregular voltage fluctuations, indicating increased interfacial heterogeneity.

The results show a clear relationship between surface morphology and voltage-noise response: non-uniform copper surfaces exhibit larger fluctuations, while uniformly electrodeposited copper surfaces display lower-amplitude signals. These findings demonstrate that EN analysis can provide direct insight into interfacial non-uniformity and can serve as a non-destructive diagnostic method for studying deposition behavior in energy-storage and conversion systems.

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Comparison of residual stress values in TiFe alloy measured by sin$^2\Psi$ and FIB-DIC techniques

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The hydride metal formation comes along with a crucial increase in the volume of the crystal lattice (up to 20 %). Such increase is associated with the formation of defects (microcracks and general embrittlement) [1]. Hydrogen induced pulverization leads to formation of fine powders with low thermal conductivity and, therefore, dramatic drop in hydrogenation/dehydrogenation kinetics. Therefore, the study of internal stress is necessary to improve the technological properties of hydrogen storage alloys. Intermetallic compounds based on TiFe are quite perspective for hydrogen storage instead of popular expensive $LaNi_5$-based alloys. TiFe-based alloys can interact with hydrogen at normal conditions with the hydrogen storage capacity up to 1.8 wt.% [2]

The ingots of the alloys were fabricated by arc melting the stoichiometric mixtures of the raw materials in an argon atmosphere purified by a Ti getter for residual gas removal. The structure, phase composition and residual stress values of the obtained materials were analyzed on a DRON-type X-ray diffractometer using CoKα radiation (λ=0.1791 nm) with carbon monochromator. Additionally FIB residual stress measurement technique with digital image correlation was used to compare with sin$^2\Psi$ technique.

XRD technique revealed an appearance of tensile stress in the obtained alloy (Fig. 1). The value of the tensile stress was found to be –192 MPa, taking the following values for calculation E=115 MPa and ν=0.3 [3]. To compare, FIB-DIC technique demonstrates much higher value to be –342 MPa, which is almost twice higher.

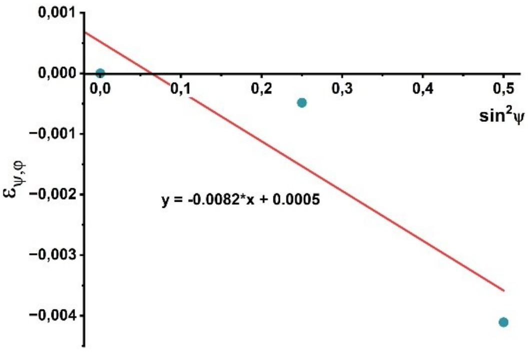

Figure 1. sin$^2\Psi$ plot for residual stress calculation.

According to [4] such difference in residual stress values can be explained by number things. First, low depth in XRD technique is highly dependent on surface stress gradient, while FIB-DIC tracks surface relaxation around the cut ring. Second, the presence of stress gradients and texture in the alloy would make difference in stress values. Moreover, in cases of elastically anisotropic behavior proper elastic modulus should be used to avoid additional sources of errors.

We suggest that in our case such high difference (almost 75%) is infused by the presence of stress gradients along the sample plane (Fig. 2). Such strongly differ in the stress value at the same depth demonstrate that FIB-DIC technique can reveal much more details about stress in the plane of the alloy, while XRD will give results only in a near-surface region. Therefore, use of both techniques would allow us to better understand the internal stresses.

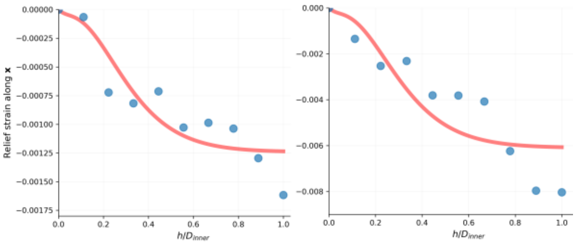

Figure 2. Grain structure image obtained during FIB-DIC analysis.

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MoS_2/Polypyrrole composites as electrocatalysts for Hydrogen Evolution Reaction

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The development of efficient and economically viable electrocatalysts for the hydrogen evolution reaction (HER) remains a central challenge in the transition toward sustainable energy systems. Among non-noble metal catalysts, molybdenum disulfide (MoS_2) has attracted considerable attention due to its favorable hydrogen adsorption properties and layered structure with various catalytically active sites. Nevertheless, its catalytic performance is often hindered by limited electrical conductivity and insufficient exposure of active sites, requiring alternative material design strategies that enhance these properties and improve its catalytic activity.

In this work, MoS_2 with a controlled morphology was synthesized using a hydrothermal method, resulting in hierarchical microspheres assembled from flower-like nanosheet architectures. This structure expose a high density of edge sites that serve as the primary active centers for the hydrogen evolution reaction. The hydrothermally synthesized MoS_2 exhibits superior catalytic performance compared to commercially available MoS_2, and was therefore chosen as a suitable starting material for further modification and optimization.

To overcome the intrinsic limitations of MoS_2, composite materials with the conductive polymer polypyrrole (PPy) were developed with the aim of improving charge transport and interfacial properties. Multiple synthesis strategies were employed to tailor the interaction between MoS_2 and PPy, including mechanochemical mixing of pre-synthesized components, incorporation of one component during the synthesis of the other, as well as simultaneous formation of both phases. These approaches enabled systematic variation of composite architecture and interfacial contact.

The electrocatalytic activity of the prepared composites toward HER was systematically investigated in acidic media. Structural and electrochemical analyses suggest that the method of composite preparation plays a critical role in determining catalytic performance. The incorporation of PPy generally contributes to improved electrical connectivity and modifies the electrochemical response of the material. The improved activity can be attributed to the combined effects of increased electrical conductivity, higher density of accessible active sites, and optimized charge transfer kinetics. In addition, the composites exhibit favorable durability and stability under prolonged electrochemical conditions, suggesting their potential for practical applications.

However, the results also indicate that the composition of the composite must be carefully optimized. While moderate incorporation of the conductive polymer enhances catalytic behavior, higher PPy content was found to adversely affect HER activity, as is shown in Figure 1, likely due to partial blocking of active MoS_2 sites or altered surface accessibility. Interestingly, an increase in polypyrrole content was associated with a noticeable expansion of cyclic voltammetry profiles, pointing to enhanced capacitive contributions and increased electrochemically accessible surface area. This observation highlights a complex interplay between catalytic activity and charge storage characteristics within the composite system. Such behavior underscores the dual functional potential of these materials - as catalysts and as supercapacitors, while also emphasizing the importance of balancing conductivity, active site availability, and surface properties.

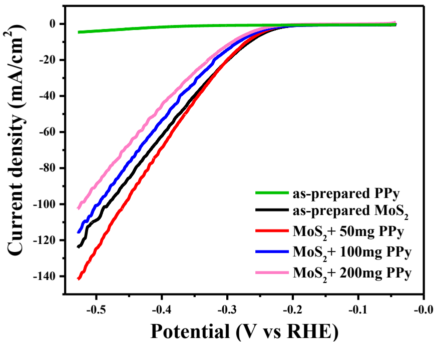

Figure 1. Polarization curves of as-prepared materials and MoS_2/PPy composites in 0.5 M H_2SO_4

Overall, this study demonstrates a viable route for enhancing the electrocatalytic properties of MoS_2 through integration with conductive polymers such as polypyrrole. The insights gained from this work provide a useful framework for the rational design of next-generation, cost-effective, and efficient catalysts for hydrogen production.

Acknowledgements

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Synthesis and Optimization of $Ti_3C_2T_x$ MXene Materials and Their Integration into PANI/MXene Composites

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MXene materials represent a modern class of two-dimensional (2D) materials obtained by the selective removal of the A-layer from corresponding MAX phases [1]. Owing to their layered structure, large specific surface area, and outstanding electrical, mechanical, and chemical properties, MXenes have attracted significant research interest, particularly in the fields of energy storage, catalysis, and sensing applications. A key challenge in their application lies in controlling the synthesis process and morphology, as these factors directly influence the final material performance [2].

In this study, the synthesis parameters of Ti_3C_2 MXene material derived from the Ti_3AlC_2 MAX phase were optimized using a molten-salt-assisted etching method followed by a post-annealing treatment (Fig. 1). The synthesis was carried out under various experimental conditions, with key process parameters varied to investigate their influence on the structural properties and phase composition of the obtained material. Particular attention was given to the efficiency of Al layer removal from the initial MAX phase, which is a crucial step in forming the characteristic layered MXene structure. The obtained samples were analyzed by X-ray diffraction (XRD), enabling monitoring of changes in the crystal structure and identification of optimal synthesis conditions for achieving desirable structural characteristics.

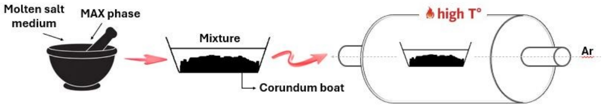

Figure 1. Schematic illustration of the molten salt-assisted synthesis of Ti_3AlC_2 MAX phase.

Based on the optimized synthesis parameters, composites based on polyaniline (PANI) and $Ti_3C_2T_x$ MXene were prepared with the aim of improving their structural and interfacial properties. The formation of PANI/MXene composites enables the combination of the conductive properties of the polymer with the unique characteristics of MXene materials. The obtained composites were further characterized using XRD and FTIR spectroscopy, confirming intermolecular interactions and the successful integration of the polymer and MXene components into a composite structure.

The results of this study indicate that optimization of synthesis parameters has a significant impact on the structure and quality of the obtained MXene material, as well as on the formation of stable PANI/MXene composites. The obtained materials provide a basis for further research toward their potential application in advanced functional and electrochemical systems.

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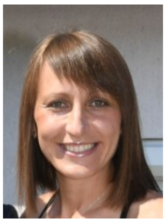

Researcher in the field of materials science, with a focus on polymer and metal-oxide materials and their composites. Engaged in their synthesis, modification, and applications in electrochemistry and photocatalysis. Particular interest is devoted to the application of machine learning in the analysis and optimization of materials. Research also includes the development of materials for hydrogen storage and their application in energy conversion.

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Shaping Georgia’s Green Hydrogen Transition: a Socio-Technical Triad Approach

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Hypothesis 1: Green Hydrogen Transition as a Socio-Technical System

The development of green hydrogen in Georgia represents a socio-technical transition in which technological potential is structurally constrained by institutional capacity and social factors. This hypothesis holds that technological progress, including the Georgian Oil and Gas Corporation's pilot projects, remains systemically constrained in the absence of an effective governance framework. Accordingly, the long-term sustainability of the transition necessitates the establishment of an integrated triadic model encompassing technology, governance, and public legitimacy.

Empirical Part (Pilot Qualitative Study, N=45) of the study is based on qualitative data from 2025 (purposive sampling: 20 experts and 25 civic stakeholders). The analysis was carried out using a qualitative thematic analysis approach, which enables the systematization of thematic categories and the identification of frequency-based estimates. 75% of respondents indicated a strategic gap between technological readiness and the absence of a National hydrogen policy framework. An information deficit in the civil sector (80%) has also been identified, which limits the formation of social support for the technological transition. This confirms the structural asymmetry between technological development, institutional framework and social awareness.

Figure 1. A Socio-Technical Triad Approach

Hypothesis 2: Social legitimacy and the energy justice dilemma

The Green Hydrogen transition in Georgia is characterized by a deficit of social legitimacy, which is due to the lack of energy justice. The weakness of the social dimension shapes the perceived as a form of “green extractivism”, where the transition is perceived as an external resource allocation rather than a local development process.

International frameworks indicate that the success of the Green Hydrogen transition depends on the integration of energy justice and social acceptance into the policy design.

Table 1. SLO and energy justice indicators

Indicator	Assessment	Perception
Local Benefits Recognition	15%	Very low

The deficit of legitimacy is manifested in the weakness of the Social License to Operate (SLO), which indicates low social trust and limited engagement. Empirically, only 15% of respondents see local benefits, which weaken the basis of social support and limits the formation of SLO. This confirms that the energy justice deficit is a systemic limiting factor of social legitimacy.

Hypothesis 3: Geoeconomic positioning and governance transformation

The geoeconomic potential of Green Hydrogen in Georgia depends on the institutional consolidation of the governance model. The existing fragmented governance structure significantly limits the country's ability to transition from a transit function to an active participant in the global energy value chain. According to empirical data, the majority of experts (65%) point to the lack of a standardized Hydrogen Governance Framework as the main determinant of investment uncertainty. This indicates that the current governance model is insufficiently integrated with international energy and regulatory frameworks. Accordingly, geoeconomic integration requires institutional consolidation of the governance system, ensuring the coordination of policy, technology and international requirements. This indicates that governance consolidation is a necessary prerequisite for Georgia’s integration into the global energy value chain.

Conclusion: Georgia’s Green Hydrogen transition reflects a three-dimensional socio-technical imbalance in which technological, social, and governance factors jointly shape transition trajectories. Its success depends on the systemic alignment of these components. The model provides a transferable framework for analyzing similar energy transitions in other emerging contexts.

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Deterministic Cost-Effective Strain Engineering of Quantum Ligth Emitters in Two Dimensional Semiconductors

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We present a cost-efficient method to create deterministic quantum emitters in two-dimensional semiconductors using localized strain induced by dielectric microparticles. The approach enables spatial control of nanoscale light sources with single photon emission and exciton biexciton cascades for quantum photonic applications.

Two-dimensional semiconductors are emerging as a powerful platform for nanoscale quantum light sources because of their strong excitonic response and mechanical flexibility. However, achieving scalable and deterministic positioning of quantum emitters remains a major challenge for their integration into photonic and optoelectronic systems.

Here, we demonstrate a lithography-free strategy to generate strain-induced quantum emitters in GaSe by transferring exfoliated flakes, using an all-dry viscoelastic stamping method, onto optically active $LiYF_4:Nd^{3+}$ bipyramidal microparticles with typical lateral dimensions of about 2 to 3 μm, which were previously randomly dispersed on the surface of Si substrates coated with a 300 nm thick SiO_2 layer. The sharp corners of these bipyramidal microparticles create highly localized strain gradients that form deep exciton trapping potentials, while the Nd3+ emission, centered around 1.436 eV, provides an optical marker that facilitates identification of the strain sites.

Low-temperature micro-photoluminescence (μ-PL) spectra measured at 10 K using a continuous wave 532 nm laser line focused to a spot of about 1.5 μm on strained regions differ strongly from those recorded on unstrained parts of the same flake, which show only broad emission characteristic of multilayer GaSe. At the strain maxima, narrow emission lines appear in the spectral range of 1.95 – 1.98 eV, spatially localized at the microparticle corners. Power-dependent μ-PL spectroscopy identifies exciton (X) and biexciton (XX) recombination from the same confined state, while polarization-resolved measurements show a common polarization axis for both transitions, thus further confirming that they originate from a single quantum confined state.

Photon-correlation experiments performed on the isolated emission lines confirm single-photon emission, with strong antibunching evidenced by $g^{(2)}(0)<0.3$ after background correction. This demonstrates that each strain induced site acts as a single photon emitter. The decay times of 1–3 ns, measured by time-resolved μ-PL, are consistent with excitonic recombination in GaSe quantum emitters. The biexciton binding energy of approximately 5 meV corresponds to an effective trap radius of about 13 nm, indicating that the strain induced charge-carrier confinement potential created by the microparticle corners acts as a true nanoscale quantum dot within the two-dimensional crystal.

Representative optical spectra, polarization and photon correlation data of the strain induced emitters are shown in Fig. 1 and discussed in Ref. [1].

Reproducible results across multiple particles and different flakes show that the brightest emitters are consistently located at the positions of maximum strain created by the microparticle corners, demonstrating that emitter formation is governed by microparticle geometry. This also indicates that emitter position and density can be controlled through engineering the shape and placement of the microparticles, providing a scalable and cost-efficient route toward the deterministic engineering of quantum light sources in layered semiconductors.

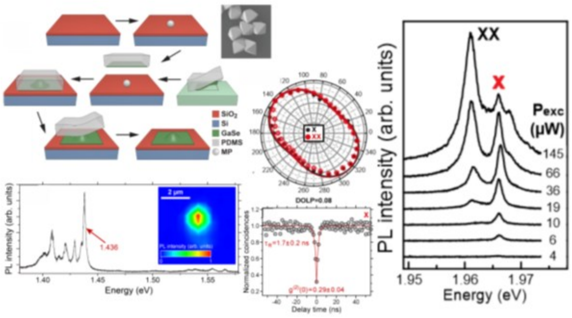

Figure 1. Fabrication and optical characterization of strain induced quantum emitters in GaSe using bipyramidal dielectric LiYF4:Nd3+ microparticles, showing localized emission, polarization, photon antibunching and exciton (X) and biexciton (XX) features.

To summarize, we demonstrate a scalable and lithography free method to engineer quantum light sources in two-dimensional materials using strain fields. This platform provides cost-efficient deterministic optical emitters for nanophotonic and optoelectronic systems based on layered semiconductors.

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Ag and Fe Alloying in Mg_2Ni Systems: Impact on Surface Composition and Corrosion Behavior

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This study examines the influence of silver (Ag) and iron (Fe) substitution on the microstructure and hydrogen storage performance of Mg_2Ni based alloys. Among magnesium based materials, Mg_2Ni has attracted considerable attention due to its relatively low hydrogenation enthalpy, favorable cycling stability, and tunable properties through alloying [1]. Compared to pure Mg, Mg_2Ni enables hydrogen absorption and desorption at lower temperatures and contributes to reducing kinetic limitations, which are a major drawback of Mg-based systems. In particular, micro- and nanostructured Mg_2Ni alloys are promising for energy storage applications due to their rapid hydrogen exchange and high storage capacity. To further enhance these properties, the present work explores the effects of Fe and Ag on surface composition and corrosion behavior under ambient exposure.

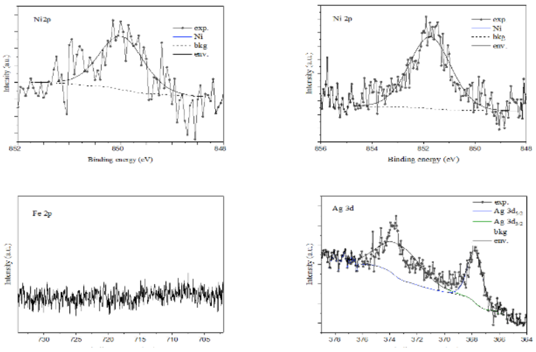

Figure 1. Experimental Ni 2p, Fe 2p, and Ag 3d XPS spectra and their corresponding fits for the $Mg_{1.95}NiFe_{0.05}$ (left) and $Mg_{1.95}NiAg_{0.05}$ (right) samples.

Surface analysis reveals distinct differences between the two alloying elements. An interesting experimental observation is that Fe, although introduced as an alloying element, is largely absent from the observable surface layer. In contrast, Ag displays a clearly visible spectral line and is found in significantly higher concentrations than initially anticipated. Nickel was detected in both samples but in smaller quantities than predicted. This observation aligns with the established understanding of surface corrosion behavior, where nickel tends to remain as a metallic phase beneath a layer primarily composed of magnesium oxide (MgO) and magnesium carbonate ($MgCO_3$) [2]. The thickness of the corrosive layer, which can reach the micrometer scale after prolonged exposure, combined with the limited information depth of the technique, undoubtedly contributes to these findings.

Table 1. Surface composition of the investigated samples.

	Relative concentration (at. %)				
	C	O	Mg	Ni	Fe/Ag
$Mg_{1.95}NiFe_{0.05}$	40.52	57.45	2.01	0.02	/
$Mg_{1.95}NiAg_{0.05}$	51.30	46.88	1.40	0.12	0.30

The XPS analysis reveals a higher contribution of oxide species on the surface of the $Mg_{1.95}NiAg_{0.05}$ sample compared to $Mg_{1.95}NiFe_{0.05}$, indicating the formation of a more defined oxide layer. In contrast, the $Mg_{1.95}NiFe_{0.05}$ sample shows a dominant contribution of species associated with hydroxyl groups and adsorbed contaminants, along with a more complex carbon chemistry.

From a corrosion perspective, these results suggest that the Ag-containing sample forms a more uniform and stable surface layer that can act as an effective passivating barrier, slowing down further surface degradation. In contrast, the Fe-containing sample exhibits a more reactive and dynamically evolving surface, which may facilitate ongoing interactions with the environment and result in reduced surface stability and less effective long-term corrosion protection.

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Desorption kinetics from MgH_2-W composites

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1. Introduction

Solid-state hydrogen storage using magnesium hydride (remains a highly attractive solution for clean energy systems due to its high theoretical capacity and excellent reversibility (1). However, its widespread industrial implementation is severely bottlenecked by slow sorption kinetics and high thermodynamic stability, which demand desorption temperatures typically exceeding. To overcome these barriers, high-energy ball milling (HEBM) is universally applied to induce severe plastic deformation, reduce grain size to the nanoscale, and introduce a high density of defects and grain boundaries that act as fast diffusion pathways. Furthermore, the introduction of transition metal catalysts has proven crucial in accelerating the recombination/dissociation of hydrogen. Among these, transition metals exhibit exceptional catalytic activity due to its multi-valence nature and ability to facilitate hydrogen transfer across the matrix interfaces (2).

While most studies focus solely on crystalline phase evolution, the structural state of the milled blend often includes a significant fraction of disordered or amorphous phases that play a vital role in the initial stages of hydrogen release. This study evaluates the synergistic effects of HEBM and tungsten addition (2 and 5 wt.%). We employ a comprehensive microstructural characterisation, including FTIR-ATR to probe the amorphous matrix components, alongside rigorous DSC-based kinetic modelling to isolate the precise rate-limiting steps governing the desorption pathway.

Commercial powder was blended with tungsten powder in two distinct concentrations: 2 wt.% and 5 wt.%. To prevent oxidation and moisture contamination, all handling, weighing, and loading of the powders were strictly performed inside an argon-filled glove box. The mixtures were processed in a high-energy planetary ball mill using hardened steel vials and balls. The ball-to-powder weight ratio (BPR) and milling duration (from 15-45 minutes) were optimized to ensure uniform catalyst dispersion and steady mechanical driving force without excessive cold welding. Phase identification, crystallite size reduction, and lattice strain variations were determined via X-ray diffraction utilising radiation. Laser particle size distribution analysis was performed in a non-polar liquid medium to quantitatively measure the geometric agglomerate size changes resulting from the milling process. Surface morphology, fracture cross-sections, and the elemental distribution of the vanadium catalyst within the matrix were observed using scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (EDS). Fourier transform infrared spectroscopy in the attenuated total reflection mode was employed in the range of to detect structural changes in the bending and stretching modes, specifically targeting the presence and behavior of amorphous or disordered species in the highly strained blends. The thermal decomposition behavior and hydrogen desorption temperatures were monitored using temperature-programmed desorption. Samples were heated from room temperature to under a continuous high-purity argon flow at various linear heating rates.

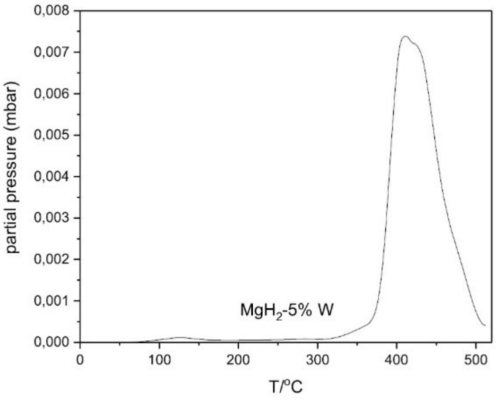

Figure 1. TPD curve of MgH_2-5%W

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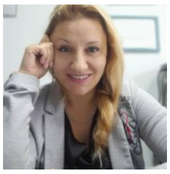

As a Senior research associate at the Vinča Institute, Sanja is committed to environmental preservation. She works on replacing fossil fuels with hydrogen through renewable energy projects, believing that the problem must be tackled at its root. Simultaneously, she is engaged in air purification and improving the air quality. Aware of the importance of green methods, she strives to replace traditional chemical syntheses with new, eco-friendly methods in every field she is involved in.

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Nickel doped rice husk activated carbon composites: Potential electrodes in H_2 generation

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Carbon–nickel (C-Ni) composite electrodes offer an alternative to conventional materials (platinum, ruthenium catalysts) for electrolytic hydrogen generation [1, 2]. In the field of electrochemical synthesis, developing new materials is increasingly critical as demand grows for cost-effective, sustainable energy technologies and circular economies.

We fabricated nickel doped rice husk activated carbon (Ni-RH-AC) composite electrodes and tested them on hydrogen and oxygen electrolytic generation via water electrolysis. Dried rice husk was impregnated with 85% orthophosphoric acid (H_3PO_4) at a 1:1 (w/w) ratio. The resulting paste was placed in an alumina crucible and heat treated at 500 °C for 2 h in an Ar atmosphere using a horizontal alumina tube furnace. After cooling to room temperature, the product was ground and washed with deionized water until neutral pH was reached. Doping with Ni was as follows: NiO mixed with RH-AC (20, 30 wt% RH-AC) was pyrolyzed in closed-loop reactor under an ethanol atmosphere at 700 °C for 1 h. During this process, NiO is reduced to metallic Ni, atoms of which nucleate on carbon defect sites and coalesce into nanoparticles. Figure 1 depicts SEM images and EDS spectra for samples of rice husk activated carbon and Ni doped RH-AC.

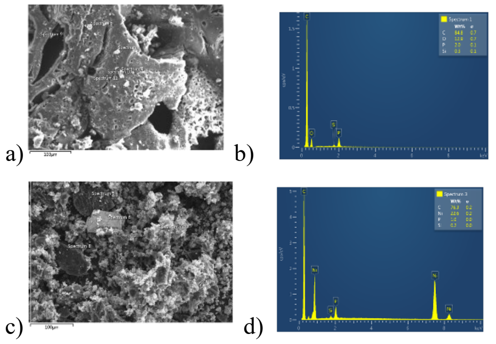

Figure 1. SEM images and EDS spectra of rice husk activated carbon before (a, b) and after doping with Ni (c, d)

The surface structure for doped Ni-RH-AC (a) is more developed compare to just rice husk activated carbon and clear Ni pick appears on EDS spectra (d).

The following electrode were prepared: (1) Ni-doped CNT on graphite electrodes with varying Ni content, (2) FTO-glass electrodes modified with a TiO_2/C/Ni/PEDOT coating using either rice-husk activated, or commercial carbon powders. Electrochemical characterization such as linear voltammetry, cyclic voltammetry and electrochemical impedance spectroscopy of prepared electrodes in alkaline solutions were used to assess intensity of the process of water electrolysis with electrochemical generation of hydrogen and oxygen gas. Preliminary measurements indicate that several of the tested Ni-RH-AC composite electrodes show promising current flows especially for oxygen evolution reaction pointing to the more favorable water oxidation process relative to Ni-doped CNT on graphite electrodes.

While full characterization is ongoing, these early trends suggest that nickel doped biowaste (rice husk) activated carbon composites may be viable cost-effective electrode materials for water splitting reaction and motivate further analysis of their properties, long-term stability, and the influence of fabrication variables on performance. We are also planning to investigate potential applications of fabricated electrodes in photoelectrochemical H_2 generation.

Acknowledgements

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X-ray Absorption Spectroscopy Study of Mg-V Thin Films for Hydrogen Storage

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Magnesium-based hydrogen storage materials attract attention because of their high gravimetric hydrogen capacity and reversible cycling properties. However, they are limited by slow hydrogenation/dehydrogenation kinetics and high operating temperatures. Different approaches, such as the addition of catalysts, mechanical milling and ion irradiation, have been widely investigated to improve hydrogen sorption properties through defect formation and modification of the local microstructure [1, 2].

Multi-edge X-ray Absorption Near-Edge Structure (XANES) approach was employed to study Mg/V thin films [3]. Room temperature XANES measurements were performed at ASTRA and PIRX beamlines of the SOLARIS National Synchrotron Radiation Center in Krakow (Poland). By employing different detection modes, namely, Fluorescence Yield (FLY) and Total Electron Yield (TEY), different regions of the films were probed. Spectra were collected at Mg and V K-edges, V $L_{2,3}$-edge and O K-edge in order to determine oxidation state, local coordination geometry and chemical environment of Mg and V in irradiated and hydrogenated Mg/V thin films. Spectra were normalized using PyMca software and subsequently processed and analyzed using ATHENA package.

Mg K-edge XANES spectra of only irradiated films resemble Mg metal with broad, weak features characteristic for Mg^0, while some irradiated and hydrogenated films resemble MgO-SiO_2 silicate glasses containing coexisting 4-fold and 6-fold Mg coordination [4], suggesting intermixing at the Mg/SiO_2 interface during hydrogen irradiation. Spectra of hydrogenated films show near-edge features characteristic for MgO, while suppression of multiple-scattering peaks in TEY mode indicates loss of long-range order and amorphization.

V K-edge XANES spectra of irradiated films differ significantly from those of irradiated and hydrogenated films. Irradiated films exhibit a lower absorption edge and weak pre-edge features characteristic for V_2O_3 phase (V^{3+} oxidation state), whereas irradiated and hydrogenated films show absorption edge shifted for more than 3 eV toward higher energies together with very strong pre-edge features characteristic for V_2O_5 phase (V^{5+} oxidation state) (Table 1.).

V $L_{2,3}$-edge XANES spectra confirm higher vanadium oxidation state in hydrogenated films through shifts of the L_3 and L_2 regions toward higher energies. Absence of pronounced pre-edge features in irradiated films indicates formation of V_2O_3 inside the films, while hydrogenated films exhibit distinctive pre-edge characteristic for V_2O_5 together with broad MgO-like main-edge features, implying coexistence of separate MgO and V oxide phases with high degree of structural disorder.

The obtained results show that hydrogenation strongly modifies the local coordination and oxidation state in Mg/V thin films, promoting oxidation of vanadium, formation of MgO-rich disordered phases, and partial amorphization.

Table 1. Vanadium oxidation state, coordination number (CN), ligand environment and the estimation of the expected pre-edge intensity in common vanadium oxides.

	V oxidation state	**CN**	**ligand environment**	**pre-edge intensity (eV)**
V metal	0	8	metallic	very weak
VO	2+	6	octahedral (centrosymmetric)	weak
V_2O_3	3+	6	distorted octahedral	moderate
VO_2	4+	6	distorted octahedral	moderate-strong
V_2O_5	5+	5	distorted square pyramidal	very strong

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Computational Screening of Li and Na Amidoborane Formation

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While ammonia borane (HAB) possesses an extraordinary theoretical hydrogen capacity, its application is limited by multi-step desorption kinetics and the formation of detrimental by-products like borazine. This study explores the transition to monometallic amidoboranes (MAB), which effectively eliminate borazine release and lower the operating temperature. Despite a slight reduction in weight percentage compared to pristine HAB, these alkali-metal derivatives offer a more viable pathway for efficient hydrogen storage.

Solid state reactions between alkali metal hydrides (LiH, NaH) and ammonia borane proceed spontaneously, yet their kinetics and phase formation pathways depend strongly on the alkali cation. We used in situ Raman spectroscopy to monitor the reactions of LiH and NaH with HAB and observed markedly different behavior, including distinct reaction rates and contrasting spatial progression of new phase formation.

To rationalize these differences at the atomic scale, we combine a universal machine learning interatomic potential (UMA MLIP) [1] with density functional theory (DFT) to investigate the early stages of interaction and the subsequent formation of Li amidoborane (LiAB) and Na amidoborane (NaAB). Initial surface adsorption structures of AB on LiH and NaH were generated using the AutoAdsorbate package [2] that automatically identifies chemically distinct adsorption motifs (e.g., on top, bridge, and multi fold environments), producing a diverse set of chemically reasonable starting configurations for subsequent structural relaxation and energy evaluation.

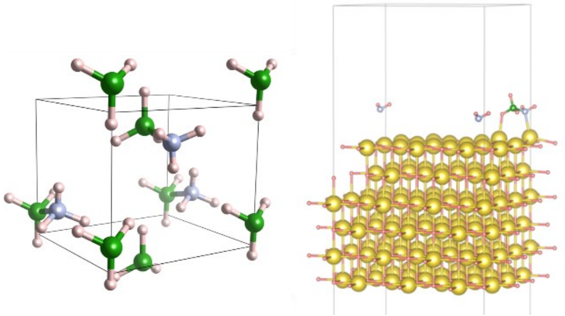

Figure 1. Crystal structure of HAB (left) and energetically favorable adsorption site of a HAB molecule on the (100) NaH surface (right). N – green, B – blue, H – pink, Na-yellow spheres.

In addition, we model the reactive interface between LiH/NaH and orthorhombic HAB to probe how interfacial structure and local chemistry steer reaction pathways. DFT calculations are further used to compute Raman spectra of HAB, LiAB, and NaAB, enabling direct assignment of experimental bands and facilitating mechanistic interpretation of measurements.

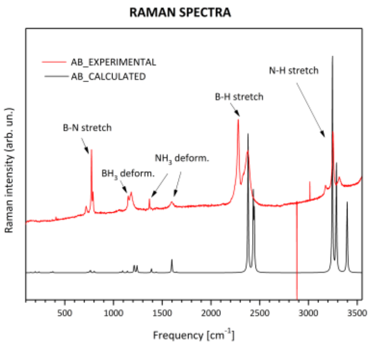

Figure 2. Experimental vs calculated HAB Raman spectra.

Together, the combined UMA MLIP/DFT workflow links observed spectroscopic signatures to atomistic reaction motifs and provides a mechanistic basis for the divergent reactivity of LiH versus NaH in solid state LiAB/NaAB formation.

Acknowledgment

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Catalytic Effects of Ni and Co on MgH_2 Hydrogen Desorption under Short Milling Times

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The effect of nickel (Ni) and cobalt (Co) additives on the hydrogen desorption properties of magnesium hydride (MgH_2) were investigated using short milling times (15, 30, and 45 minutes). The incorporation of Ni significantly reduced the hydrogen desorption temperature by more than 100 °C compared to the pure MgH_2 [1]. Kinetic analysis indicated that hydrogen desorption in Co-doped samples follows Avrami-Erofeev model (n=4), with the apparent activation energy (Ea) decreasing with increasing milling time and additive content.

Table 1. The ratios and quantities of desorbed hydrogen from TPD profiles.

	LT peak (%)	HT peak (%)	Ratio (LT/HT)
$MgH_2$10Co15	29	71	0.41
$MgH_2$10Co30	31	69	0.45
$MgH_2$10Co45	53	47	1.13
$MgH_2$20Co15	39	61	0.64
$MgH_2$20Co30	62	38	1.63
$MgH_2$20Co45	77	23	3.38

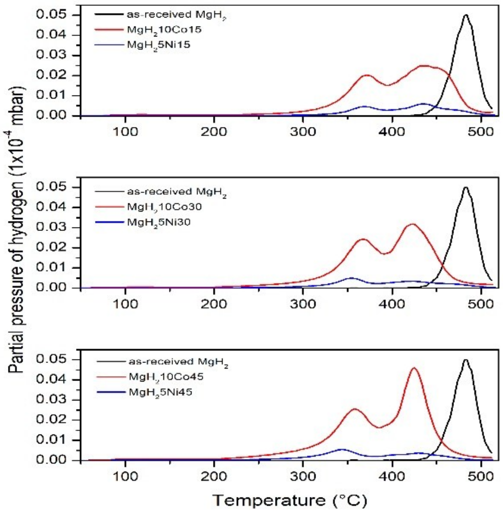

Figure 2. TPD curves of milled MgH_2 with 10 wt.% Co compared to the milled MgH_2 with 5 wt.% Ni and as-received MgH_2.

The MgH_2-Co composite containing 20 wt.% Co, milled for 45 minutes, exhibited the best desorption performance, with a low-temperature (LT) maximum at 310°C and an LT/HT ratio of 3.38 (Table 1). In systems with Ni and Co, the catalytic contribution of transition metals was identified as the dominant factor enhancing hydrogen release, while the effect of mechanical grinding was less pronounced. These findings suggest that mechanochemical processing involves two distinct contributions – mechanical refinement and catalytic activity – with the latter playing a more significant role at shorter milling times.

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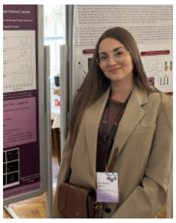

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Machine learning-assisted, literature-based screening of high-entropy alloys for solid state hydrogen storage

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In recent years, the high-entropy alloys (HEAs) have emerged as a particularly promising class of candidate materials for hydrogen storage. However, their vast combinatorial composition space is far beyond what conventional trial-and-error synthesis can explore, making exhaustive experimental screening or first-principles simulations impractical. This overload of potential motivates a machine learning-based approach to materials screening to help identify thermodynamically favorable hydride-forming compositions. However, the missingness rate of reported physicochemical properties varies greatly by material class across different data sets. This leaves a high proportion of unreported labels, which inhibits predictions of target properties. Accordingly, machine learning-based predictions now often rely on text-derived chemical element or materials representations in format or word embeddings [1]. These embeddings offer feature representations that capture the chemical context found in published texts [2].

In this work, we present an end-to-end screening framework that combines data from multiple first-principles databases (Materials Project, AFLOW, and JARVIS-DFT) to assemble a training set of a great variety of materials. Each material is described by its inherent structural parameters and DFT-computed formation energy. In addition, we constructed composition-based feature vectors using the matminer library to capture materials descriptors, including valence-electron concentration, atomic radius mismatch, electronegativity variance, and d-band proxies relevant to hydrogen binding. The dataset is used to screen a systematically constructed virtual library of HEA compositions based on established systems, identifying candidates that satisfy thermodynamic windows for reversible hydrogen absorption near ambient conditions. Word embeddings trained on a materials science corpus are pooled by several different criteria into composition-level features and concatenated with classical phase-stability descriptors [3, 4], together with binary missingness indicators on the descriptors themselves. In contrast to predictive positioning of materials using combined descriptors and text-based representations, the similarity-based materials analysis operated in the feature space rather than the label space. The trained predictor scored phase-stable equiatomic candidates enumerated from a data-driven pool of chemical elements and annotated with predicted properties.

In addition to sparse property selection, the limitations of the current work stem from the fact that text-derived embeddings supporting predictive behavior inherit publication bias. Namely, chemistries investigated in greater detail have rich vector representations, while those neglected or underrepresented receive sparse vectors or very low-quality representations. We further discuss how explicit label-side and feature-side missingness affects predictive calibration and discovery, and how it generalizes to other materials informatics tasks where literature corpora and labeled databases coexist with structurally non-random gaps.

The results demonstrate the potential of high-throughput computational screening combined with interpretable machine learning to accelerate the identification of novel HEA-based hydrogen storage materials, providing prioritized targets for experimental validation.

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Effects of 3d metal doping on local and electronic structure of CeO_2 nanopowders

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The electronic structure and redox behavior of transition metal–doped CeO_2 nanopowders, were investigated by X-ray Absorption Near Edge Structure spectroscopy. Depth–resolved analysis shows that the surface is more reduced than the bulk in all samples except pristine CeO_2, whose surface is re–oxidized. These findings provide direct spectroscopic evidence of cation–defect interactions and highlight the importance of depth–sensitive techniques for understanding mixed-valence behavior and defect chemistry in TM–doped ceria systems.

Cerium oxide (CeO_2) nanoparticles are widely used for energy storage due to the reversible Ce^{4+}/Ce^{3+} redox couple, high oxygen storage capacity, and large dielectric constant, enabling their application as electrode materials in supercapacitors and as anodes in lithium–ion batteries [1]. Incorporating transition–metal (TM) dopants is a key strategy to improve their performance in energy storage and conversion, as it introduces oxygen vacancies and tailors the electronic band structure. These changes enhance ionic conductivity, boost redox activity, and extend light absorption into the visible region [2].

In this work, high purity ultrafine CeO_2 nanopowders with 4 wt.% TM (TM = Fe, Co, Ni, Cu, Zn), synthesized by self–propagating combustion glycine–nitrate process [3], were studied by X – ray Absorption Near Edge Structure (XANES). Measurements were performed at SOLARIS National Synchrotron Radiation Center in Krakow (Poland). To separately probe the surface and the near–surface region, spectra were collected in Total Electron Yield (TEY) and Fluorescence Yield (FLY) modes. Cerium $M_{4,5}$–edge XANES spectra are highly sensitive to the 4f orbital occupancy that governs the material's redox properties. The oxidation state of cerium can be clearly distinguished by its different spectral signatures – Ce^{3+} ($4f^1$ ground state) is dominated by lower energy features A, B and C (A', B' and C'), whereas Ce^{4+} ($4f^0$ ground state) exhibits a complex multi–peak structure (features D, E and D', E') at higher energies (see Fig. 1).

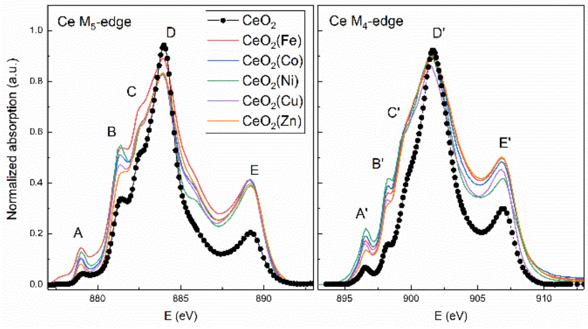

Figure 1. Ce $M_{4,5}$ XANES spectra collected in TEY mode.

The M_5/M_4 intensity ratio (branching ratio) derived from the integrated area under the corresponding curves (see Fig. 1), is presented in Fig. 2. Branching ratio is a critical quantitative indicator of the cerium oxidation state and 4f orbital occupancy. As can be seen form Fig. 2, branching ratios of all TM–doped samples lay in the region where mixed Ce^{4+}/Ce^{3+} is expected (region between the two horizontal lines). Also, the fraction of Ce^{3+} increases in the surface region (TEY mode) in all samples, except pristine CeO_2.

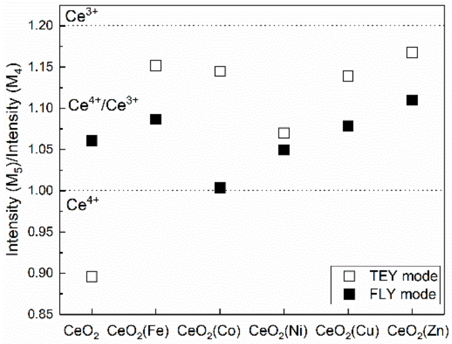

Figure 2. Branching ratio of the investigated samples in TEY and FLY modes (see text for more details).

The subsequent analysis of XAFS data collected at O K–edge and TM $L_{2,3}$–edges, together with the results obtained by complementary techniques (XRD, Raman, XPS, …), is expected to provide a comprehensive insight into the effects of TM doping on the electronic properties and defect chemistry of cerium oxide nanopowders.

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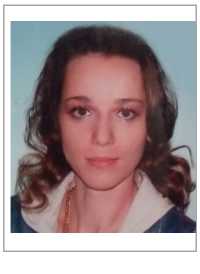

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3D Architected Laser-Induced Graphene Electrodes via Printable Polyimide Ink for High-Performance Thin-Film Supercapacitors

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Laser-induced graphene (LIG) is a promising platform for flexible thin-film supercapacitors; however, conventional approaches based on Kapton substrates fundamentally limit thickness control and hinder the realization of multilayer and three-dimensional (3D) architectures due to restricted laser penetration and poor structural tunability [1–2].

Here, we present a scalable strategy for thickness-engineered 3D LIG electrodes enabled by printable polyimide ink as a tunable precursor. This approach provides (i) precise control over film thickness, (ii) selective and conformal deposition onto pre-patterned substrates, including electrical circuits and current collectors, and (iii) straightforward multilayer fabrication for vertically integrated architectures with increased active material loading. These capabilities overcome key limitations of conventional LIG systems and enable structurally programmable electrode design.

To support mechanically robust and highly conductive multilayer architectures, a graphene oxide–eutectic gallium–indium (GO@EGaIn) composite is introduced as a compliant current collector. The composite is synthesized via ultrasonication, where graphene oxide stabilizes liquid metal microdroplets, followed by laser-induced reduction to enhance electrical conductivity and interfacial integrity.

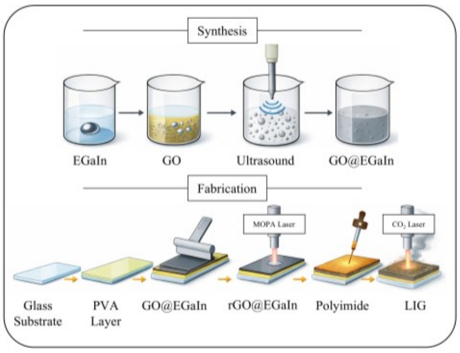

Figure 1. Schematic illustration of the layer-by-layer fabrication process for 3D multilayer LIG electrodes, including sequential deposition of GO@EGaIn current collectors and printable polyimide ink, followed by laser-induced conversion into porous graphene architectures.

The fabrication workflow consists of sequential deposition of GO@EGaIn and printable polyimide ink layers, combined with a sacrificial poly(vinyl alcohol) (PVA) layer for device transfer. Each polyimide layer is selectively converted into porous LIG via CO_2 laser irradiation, yielding vertically integrated architectures with interconnected conductive pathways (Fig. 1). Structural characterization confirms well-defined multilayer interfaces and hierarchical porosity, enabling efficient ion transport.

Electrochemical measurements (6 M KOH, symmetric configuration) demonstrate an areal capacitance of 232 mF cm^{-2} at 1 mA cm^{-2}, with stable and symmetric charge–discharge behavior (Fig.2). The performance arises from a hybrid charge storage mechanism combining electric double-layer and pseudocapacitive contributions, driven by synergistic interactions between LIG and GO@EGaIn [3].

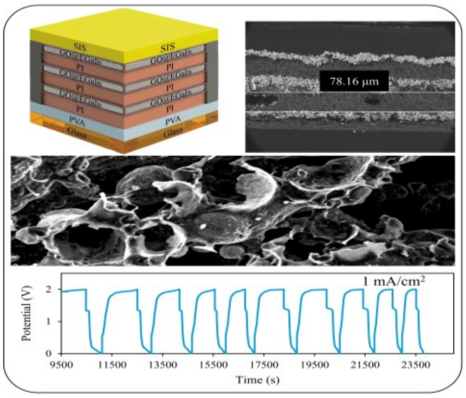

Figure 2. Structural and electrochemical characterization of the multilayer LIG electrodes: (a) 3D architectural schematic, (b) cross-sectional SEM image, (c) surface morphology, and (d) galvanostatic charge–discharge (GCD) performance.

Overall, this work establishes a scalable and structurally versatile platform for 3D architected LIG electrodes, providing a clear pathway toward high-performance, miniaturized energy storage systems.

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Liquid-Assisted Mechanochemical Formation of $CsCuCl_3$: Insights from Machine Learning Potentials and DFT

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$CsCuCl_3$ perovskite, a thermally stable and redox-active halide, is a promising candidate for energy conversion and storage applications [1] due to its ionically conductive channels, Cu^{2+}/Cu^{+} redox activity, and tunable semiconducting properties. $CsCuCl_3$ perovskite is efficiently synthesized from $CuCl_2$ and CsCl via liquid assisted grinding (LAG), using dimethyl sulfoxide (DMSO) as a minimal additive, highlighting a sustainable and scalable route to halide perovskites.

In this work we utilize atomistic simulations combining DFT and universal machine learning potential to reveal the role of solvent-mediated Cu^{2+} coordination in perovskite formation. Surface-driven reaction pathways were modeled using a pretrained OC20-compatible universal machine learning interatomic potential (UMA) within the ASE framework [3], enabling efficient sampling of adsorption at reactive interfaces. Interaction of DMSO with 10-1 surface of CuCl2 is investigated on using 3x3 slab model (Figure 1)

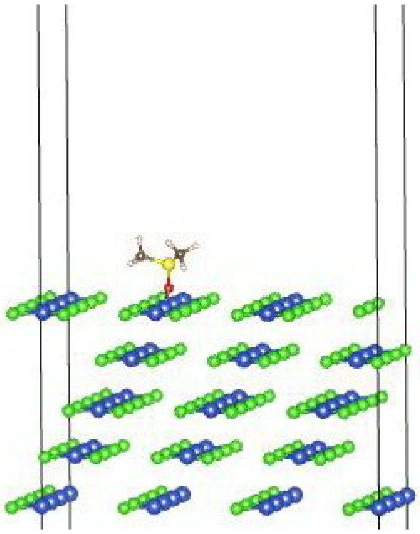

Figure 1. Interaction of DMSO with 10-1 surface of CuCl2.

Complementary density functional theory calculations at B3LYP/ 6-311++G(2d,2p) level of theory using Gaussian 09 program [4] package provide electronic structure insight into Cu–DMSO coordination (Figure 2) and charge redistribution, confirming ligand-induced weakening of Cu–Cl interactions. Mechanochemical experiments validate accelerated formation of $CsCuCl_3$ in the presence of DMSO, supporting a solvent-assisted ion rearrangement mechanism. This work demonstrates how surface-focused machine learning potentials, combined with electronic structure calculations and experiment, can provide mechanistic insight into complex solid-state reactions under mechanochemical conditions.

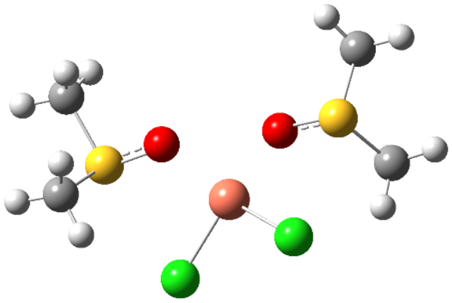

Figure 1. Structure of $CuCl_2$ coordinated with two DMSO molecules.

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The importance of quantum mechanical models to explain hydrogen evolution

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Advancing water electrolysis is key to the hydrogen energy transition, with the hydrogen evolution reaction (HER) at its core. Despite its simplicity, HER has been studied for over a century, focusing on how a proton transfers from a donor (water, hydronium, or acid) to the electrode or catalyst. Understanding has evolved from early phenomenological models to modern quantum approaches that include proton tunneling and electron–nucleus coupling.

In the present day, we understand that HER is a complex quantum-mechanical process. Key milestones along this path include: • Classical kinetics (Volmer-Tafel-Heyrovsky): defined the process's stage-by-stage nature; • Marcus theory: introduced the concept of solvent reorganization as the main source of activation energy; • Dogonadze-Kuznetsov-Levich (DKL) theory: first applied quantum mechanics to the proton, explaining tunneling and isotope effects; • Concerted Proton-Electron Transfer (CPET) theory (Hammes-Schiffer): combined electron and proton transfer in a single, coordinated event, essential for describing modern catalysts.

While Marcus's theory treated the electron as a quantum particle, and the nuclei and solvent according to classical definition, this was insufficient for the proton, which is heavier than the electron but lighter than ordinary ions. In the 1960s, V.G. Levich, R.R. Dogonadze, and A.M. Kuznetsov developed a consistent quantum theory of proton transfer [1], which became the basis for understanding cathodic hydrogen evolution. While acidic electrolysis (PEM) depends on scarce platinum-group metals, alkaline electrolysis (AEL) can use cheaper nickel and iron but suffers from HER kinetics that are 2–3 orders of magnitude slower. This slowdown is explained by the quantum-mechanical framework of Dogonadze–Kuznetsov–Levich [2], which accounts for proton–electron transfer at the electrode. The theory clarifies the unusually large hydrogen/deuterium isotope effects that classical models cannot explain [3]. It also introduced both stepwise and concerted proton–electron transfer mechanisms, anticipating modern CPET concepts.

In electrochemical kinetics, theoretical developments have often outpaced experimental confirmation. Here, we will examine examples of the application of the quantum-mechanical DKL theory of proton transfer to current problems in electrochemical hydrogen production.

In the work of Nazmutdinov et al. [4], it was shown that modern calculations using density functional theory (DFT) and molecular dynamics confirm the main conclusions of the LDC for the discharge of the hydronium ion on a mercury electrode. This unified quantum rate theory (Quantum Rate Theory) was developed. This complex reaction has attracted attention for many years, and microscopic modeling finally confirmed the previously made theoretical conclusion about the proton transfer from excited energy levels as the key effect leading to the famous Tafel plot over a wide overpotential region.

Modern strategies for creating catalysts for "Green" hydrogen directly or indirectly rely on the DKL theory provide a framework to understand how the reaction rate of HER is influenced by factors like overpotential, pH, and the nature of the electrode material. The theory has been used to predict and explain the dependence of the activation energy on the total reorganization energy of the system, which is a key parameter in understanding electrocatalytic activity. It helps to explain why certain materials are more active catalysts for HER than others, and allows calculation of the reorganization energy, required to re-arrange the solvent molecules and the internal structure of the reactants and products during the charge transfer [5]. For HER, this can be broken down into two components: the solvent reorganization energy and the reorganization energy of the discharging species (e.g., a water cluster). Researchers have applied the theory to calculate these values for HER on various metal alloys, such as molybdenum with iron subgroup metals (Fe, Co, Ni), to understand how the catalyst and solvent affect the reaction rate [6].

The current stage of theoretical development is characterized by a striving for unification. As shown in the recent work of Bueno [7], there is a deep connection between the classical Marcus theory, the quantum theory of the LDC, and modern concepts of quantum coherence.

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Flexible 2D Layered Oxide Thin Films for Solid-State Hydrogen Storage

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Hydrogen is a key energy vector for enabling a low-carbon energy system; however, its storage remains a major technological bottleneck. Conventional approaches rely on compressed gas (350–700 bar) or cryogenic liquid hydrogen, both associated with safety concerns and high energy costs. Solid-state hydrogen storage offers an attractive alternative, yet scalable and reversible material platforms are still needed.

Here, we report on **α-MoO_3 thin films deposited by plasma-enhanced atomic layer deposition (PEALD) directly onto flexible, rollable mica substrates**, enabling a new class of conformal, bendable solid-state hydrogen storage architectures (Figure 1). The use of mica is particularly advantageous due to its thermal stability, mechanical flexibility, and compatibility with high-quality ALD growth, allowing uniform thin films over large-area and non-planar geometries.

Figure 1. Concept of rollable solid-state hydrogen storage device.

The layered structure of α-MoO_3, composed of MoO_6 octahedral bilayers separated by van der Waals gaps, provides intrinsic sites for hydrogen insertion [1]. Hydrogen loading is achieved via **room-temperature H_2 plasma treatment (200 mTorr)**, enabling hydrogen incorporation under mild conditions compatible with flexible substrates. Grazing-incidence X-ray diffraction (GIXRD) reveals a systematic expansion of the *b*-axis, consistent with hydrogen insertion within the van der Waals gaps, while complementary ToF-SIMS depth profiling on films grown on mica shows a progressive increase in hydrogen signal intensity across the film thickness from 0 to 48 min of H_2 plasma exposure (Figure 2). A volumetric hydrogen storage capacity of ~28 kg·m^{-3} is achieved, comparable to compressed hydrogen storage systems, but without high-pressure operation (see Table 1). Importantly, the hydrogenation process is fully reversible, with complete desorption obtained at 350 °C under inert atmosphere and stable cycling over multiple absorption/desorption cycles.

The deposition approach is inherently scalable, and enables **precise thickness control, excellent conformality, and integration on flexible supports**, making it particularly suitable for **rollable and modular hydrogen storage devices**.

While atomistic calculations support hydrogen insertion at oxygen sites within the crystal structure, the experimental evidence highlights that **processing conditions and thin-film architecture are the dominant factors governing storage performance**.

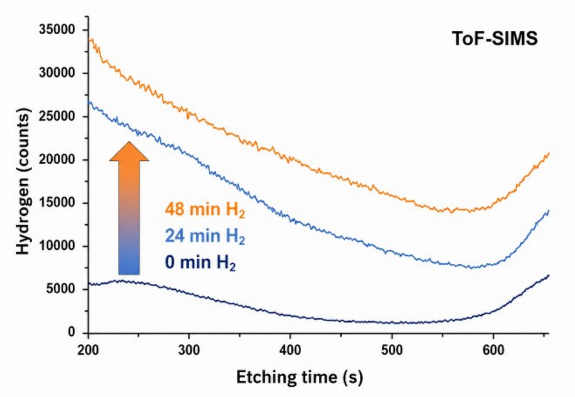

Figure 2. ToF-SIMS hydrogen depth profiles of α-MoO_3 thin films deposited on mica substrates after H_2 plasma treatment (0, 24, and 48 min).

Table 1. Comparison of hydrogen storage technologies.

Technology	Operating Conditions	Volumetric Capacity (kg H_2 m^{-3})	Key Advantages	Limitations
Compressed H_2	350-700 bar	23-40	Mature technology	High pressure, Safety issues
Liquid H_2	-252.8 °C	~70	High capacity	Cryogenic losses, energy intensive
Metal hydrides	High T / P	90-150	High storage capacity	Cost, heavy, slow kinetics
α-MoO_3 thin films (this work)	**RT H_2 plasma / 350 °C desorption**	**~28**	**Low pressure operation, reversible, flexible substrates**	**Optimisation of plasma time and thickness**

Overall, this work demonstrates that **ALD-grown α-MoO_3 thin films on rollable substrates represent a viable route toward flexible, low-pressure, and scalable solid-state hydrogen storage technologies**, bridging materials design and device integration.

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Tandem Copper - Cobalt Phthalocyanine Electrodes Enable Enhanced Electrochemical CO₂ Conversion to Ethylene

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Achieving selective multi-carbon (C_2^+) products in electrochemical CO_2 reduction (ECR) remains challenging due to competing reaction pathways. Tandem catalyst architectures have emerged as an effective strategy to address this limitation by spatially separating CO generation and subsequent C–C coupling steps [1]. Controlling reaction pathways toward multi-carbon (C_2^+) products remains a major challenge. Tandem electrode architecture has recently attracted significant attention as an effective strategy to address this challenge by spatially separating reaction steps [2]. Integrating an effective CO-generating catalyst into architecturally designed gas diffusion electrodes represents a promising pathway for improving tandem catalyst performance [3].

Electrochemical measurements of the cobalt phthalocyanine (CoPc) electrodes revealed that a higher carbon black (CB) content led to FEs of up to 90% for CO at relatively low overpotentials, corresponding to current densities between -10 and -50 mA cm^{-2} and -0.56 to -0.9 V vs. RHE, while suppressing hydrogen evolution to approximately 10%. In contrast, electrodes prepared with lower CB loading exhibited slightly reduced CO selectivity but maintained stable FEs throughout the measurements. The combination of lower CoPc loading and higher CB content likely promoted improved catalyst dispersion and greater accessibility of Co-N_4 active sites. This observation is consistent with previous reports, which attribute with decreased catalytic efficiency at higher metal phthalocyanine loadings to aggregation effects that limit active site utilization. Based on its superior CO selectivity, lower hydrogen evolution, and stable electrochemical performance, the 1 to 10 ratio of CoPc to CB was chosen for subsequent tandem electrode studies.

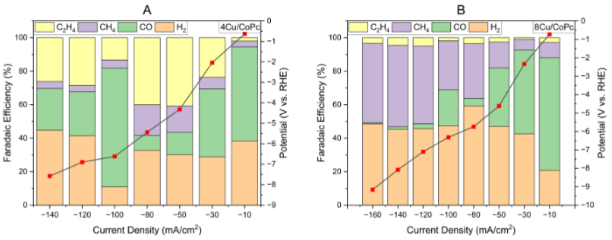

Figure 1: Different loadings of Copper - CoPc tandem electrode's FEs.

Copper electrodes were investigated following the CoPc studies to optimize sputtered copper loading, film thickness, and Nafion content for improved electrochemical performance.

The effect of copper loading and film morphology on product selectivity was subsequently evaluated to provide a reference for tandem electrode construction. Notably, lower copper loadings of 0.4 mg cm^{-2}, favored ethylene formation, achieving ethylene Faradaic efficiencies of approximately 20%. Whereas increasing the metal loading to 0.8 mg cm^{-2}, induced a transition toward methane-dominated pathways. This shift is likely associated with changes in local CO coverage and surface reaction environments that influence intermediate binding energies and proton-coupled electron transfer pathways. Based on these findings, 30 µl Nafion layered with 0.4 mg cm^{-2} copper loaded electrode was selected as the optimal platform for subsequent tandem electrode fabrication. Fabricated tandem electrode properties are given in the Table 1.

Table 1. Fabricated tandem electrodes specifications

	Cu loading (mg)	**Area of Electrode (cm^2)**	**Nafion amount (µl)**
4Cu/CoPc	0.4	1	30
8Cu/CoPc	0.8	1	30

The electrochemical results revealed clear loading dependent selectivity trends in the tandem electrodes. 4Cu/CoPc, incorporating a lower sputtered copper loading, favored ethylene formation and achieved FEs of approximately 40% at current densities of 50 and 80 mA cm^{-2} (Figure 1A). In contrast, the higher copper loading configuration (8Cu/CoPc) exhibited a pronounced shift toward methane production, with FEs exceeding 50% (Figure 1B). These findings underscore the critical role of copper loading in governing product selectivity and demonstrate the importance of catalyst design for targeting specific reaction pathways in tandem architectures.

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Optimal control on a single stage metal hydride hydrogen compressor: A Pontryagin minimization approach

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Metal hydride hydrogen compressors (MHHC) show promising application potential on various occasions. A single-stage MHHC cycle consists of four stages: hydrogen absorption, heating, hydrogen desorption, and cooling. Currently, research on improving MHHC performance mainly focuses on three areas: modifying hydrogen storage materials, developing novel reactor structures, and optimizing system operation[1]. In terms of operation, traditional control strategies generally trigger stage transitions based on state thresholds, e.g. reacted fraction, reaction rate. However, under a fixed constraint of total cycle time, these heuristic methods struggle to globally optimize the overall thermodynamic performance. Pontryagin's Minimum Principle (PMP) provides a solution for the operational control of highly nonlinear systems like MHHCs, which transforms the complex global time allocation into a transient Hamiltonian minimization problem[2]. Integrating the entropy generation analysis from finite-time thermodynamics (FTT) into the PMP control framework, allows for a compromise between output power and irreversible losses. The integration is a crucial step in developing a system-level theory for dynamic operational optimization[3].

In this study, a transient 0-D lumped model for a $LaNi_5$ single-stage MHHC is built. Under a fixed total cycle time, a PMP-based multi-stage optimization strategy is proposed, where the average bed temperature and average density are chosen as state variables, and the mass flow rate of the heat transfer fluid is chosen as the control variable. Within the FTT framework, an ecological-like optimization objective J is defined to characterize the trade-off between system output power and irreversible entropy generation. The objective function is expressed as follows:

$$\min_{u(t)} J = \int_0^{t_{cycle}} \left(T_0 \dot{S}_{gen}(x,u,t) - \dot{W}_{out}(x,u,t) \right) dt \qquad (1)$$

Where the transient entropy generation rate $\dot{S}_{gen}$ covers the irreversible losses caused by heat transfer at the reactor wall, flow resistance of the heat transfer fluid, and reaction kinetics. Limited by the lumped model, the entropy generation caused by internal heat transfer within the reactor bed is not considered.

A Hamiltonian function is constructed as:

$$H(x,u,\lambda,t) = L(x,u,t) + \lambda^T f(x,u,t) \qquad (2)$$

By solving the extremum condition $\partial H / \partial u = 0$, the optimal trajectory of the heat transfer fluid mass flow rate is determined.

In the indirect PMP optimization, the initial costate values are extremely sensitive and prone to local optima. A hybrid optimization algorithm combining a Genetic Algorithm (GA) and the PMP indirect shooting method is developed. The GA uses its global search capability to identify the initial costate range within a wide search space.

Figure 1 and Table 1 present the optimization results of the algorithm for a single metal hydride cycle. The variations in heat transfer fluid mass flow rate and the correlation between reaction rate and temperature show good agreement. The consistency of the initial and final cycle states ensures cycle stability.

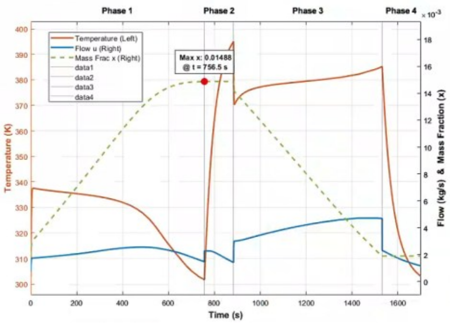

Figure 1. Optimization results for cycle time of 1700 s

Table 1. States of each stage in the hydrogen absorption-desorption cycle

	Time/s	T/K	P/bar	Frac
Start	0.00	303.00	2.9395	0.00190
Abs	756.50	301.67	3.8879	0.01488
Heat	883.37	395.00	37.6948	0.01488
Des	1531.22	385.22	21.4986	0.00190
Cool	1700.00	303.00	2.9399	0.00190

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Machine learning for hydrogen production via water splitting

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Photocatalytic and photoelectrochemical water splitting (WS) offer sustainable pathways for green hydrogen production, which is an excellent energy carrier for solar energy utilization. However, the better photocatalysts (semiconductor and co-catalyst pairs) should be developed for the commercialization of this promising technology as the efficiency suffer from the low visible energy utilization and high charge recombination rates of current photocatalysts. Machine learning/artificial intelligence (ML/AI) tools can contribute for the improvement of catalytic/photocatalytic processes, including WS reaction as part of the efforts for sustainable energy future.

ML/AI can be used in various steps of catalyst developments from initial selection of catalyst materials to designing and operating catalytic reactors as described in Figure 1 [1]. Even though catalysis research often starts with a known materials with proven performance and proceeds with some modifications, this is not sufficient for the reaction like photocatalytic WS, for which no commercially sufficient photocatalyst has been developed yet. In such cases, potential candidates are screened first; ML/AI tools can make significant contribution in this stage analyzing both experimental and computational data created in house or extracted from external sources. For the second stage, where the performance is tested, the ML/AI models can help to understand the effects of catalyst properties and operational conditions, and optimized the catalyst. This is followed by reactor design and optimization, for which various ML/AI techniques including physics informed ML for kinetics and transport limitations, and monitoring and control of the industrial scale processes.

This presentation summarizes the use of ML/AI in various steps of catalyst photocatalyst processes and provides examples for photocatalytic water splitting especially the works involving the performance analysis of photocatalytic processes to identify the importance of photocatalyst materials and properties. The challenges, opportunities and possible future direction on the subject will be briefly discussed.

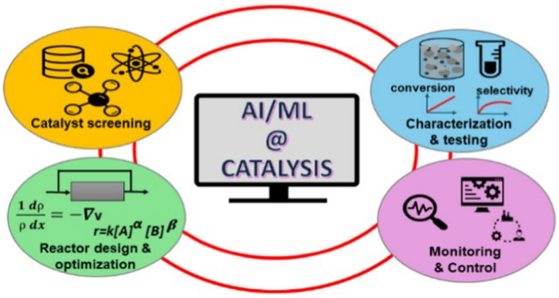

Figure 1. ML/AI framework for catalysis/photocatalysis research [1]

As an example, Figure 2 shows the parity plot for Random Forest prediction of hydrogen production rate for photocatalytic WS over halide perovskites, which are investigated extensively in recent years [2], after their remarkable success in photocatalytic applications. The dataset was contained 498 entries acquired 67 experimental studies published in the literature; the structure and composition of halide perovskite, synthesis methods, cocatalysts, cocatalyst deposition methods, reaction conditions, illumination details were used as descriptors while the total hydrogen formation rate was taken as the output variable [3].

The model predictions were generally satisfactory as evident from the RMSE values of 0.39 ($R^2 = 0.89$) for training and 0.52 ($R^2 = 0.83$) for testing. The cocatalyst type was found to be the most dominant variable, demonstrating the strongest positive SHAP values among all features.

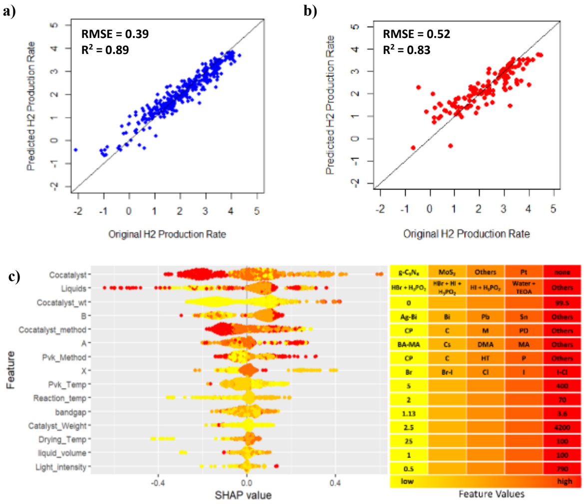

Figure. 6. Random Forest prediction of H_2 Production Rate (a) training, (b) testing, (c) SHAP analysis [3]

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Influence of convex enclosure structure on thermal discharge process of PCM

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Introduction

Phase change materials (PCMs) are widely used for thermal energy storage because they can store large amounts of heat at nearly constant temperature. However, their low thermal conductivity limits charging and discharging rates, reducing overall heat transfer efficiency. Previous studies show that curved walls can enhance heat transfer inside enclosures [1,2]. Therefore, in this study, a convex-trapezoid enclosure with curved side walls and a cylindrical obstacle is analyzed for PCM thermal discharge and compared with an isosceles trapezoidal enclosure of equal volume.

Methodology and numerical procedure

The geometries investigated in the present work are depicted in Figure 1. The bottom and top walls of the enclosures are respectively 20 and 10 mm, while the diameter of the cylindrical obstacle is 5 mm. The heights of the enclosures are different to satisfy the same PCM amount inside the enclosure for a fair comparison. In addition to that, the cylindrical obstacle location has been shifted to 5 mm upper and lower directions in vertical axis to investigate the location effects in convex enclosures.

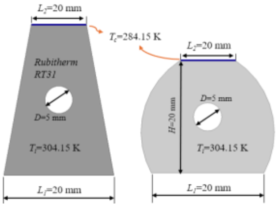

Figure 1. Investigated PCM enclosures: standard isosceles trapezoidal (left) and convex-trapezoid cavity (right).

A paraffin-based PCM (Rubitherm RT31) was used in the simulations, and its thermophysical properties are available in [3]. Density of the PCM was treated by Boussinesq approximation, while other properties are taken as constant.

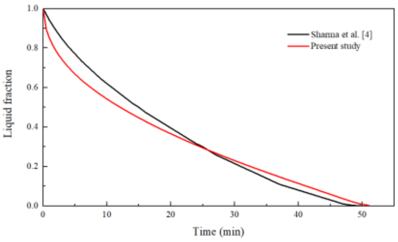

Figure 2. Validation results.

The finite volume method with the enthalpy-porosity approach was used for simulations. The model was validated by comparison with a numerically and experimentally verified study [4], showing good agreement with less than a 2-minute difference in total solidification time (Figure 2). Grid and time-step independence analyses resulted in a 150×150 grid and a 0.5 s time step, respectively.

Results and discussion

Quantitative results are presented in terms of liquid fraction evolution curves in Figure 4. Thermal discharge was completed in 308 min for the reference enclosure when the obstacle is in the middle, while this duration was only 174 min for the corresponding convex enclosure, indicating a reduction of time by 43.5%. When the obstacle is shifted to upper region, the total solidification time was found to be 192 min, while it was 166 min when the obstacle is in the lower region.

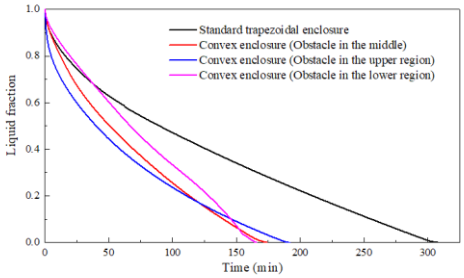

Figure 3. Liquid fraction evolutions of different cases.

Conclusion

These outcomes indicate the significance of convex wall geometry in the acceleration of thermal discharge, reaching up to 43.5% shortening in time. Hence, improvements in the enclosure design in a way that accelerates natural convection currents can be recommended as a simple yet effective technique to improve thermal discharge.

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Mg-rich High Entropy Alloy as a Rare-Earth-Free Anode Material for Ni-MH Batteries and Hydrogen Storage Applications

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The increasing demand for efficient and sustainable energy storage systems has driven research toward advanced rechargeable batteries, particularly Ni–MH systems. The performance of these batteries is largely determined by the hydrogen storage capability of the anode material. Conventional alloys, such as rare-earth-based AB_5 systems (e.g., $LaNi_5$), offer good kinetics but suffer from high cost and limited sustainability. Mg-based alloys provide high theoretical capacity but face challenges such as poor cycling stability and corrosion in alkaline environments. High entropy alloys (HEAs) have emerged as promising alternatives due to their multicomponent nature, tunable properties, and potential for improved hydrogen storage and electrochemical performance. In this study, a Mg-rich, rare-earth-free HEA was designed to combine high capacity with improved stability and cost-effectiveness for Ni–MH battery applications [1].

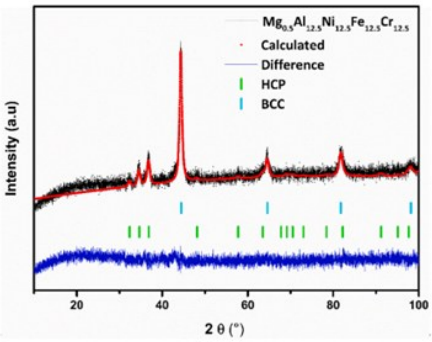

Figure 1. Powder XRD pattern of the arc-melted $Mg_{0.5}Al_{12.5}Ni_{12.5}Fe_{12.5}Cr_{12.5}$ high-entropy alloy, indicating the formation of a single-phase solid solution structure with a slight amount of HCP phase.

The $Mg_{0.5}Al_{12.5}Ni_{12.5}Fe_{12.5}Cr_{12.5}$ high-entropy alloy was synthesized using vacuum arc melting (VAM) under an argon atmosphere. To minimize Mg evaporation, a lamination strategy was applied, placing Mg at the center and surrounding it with higher melting point elements (Cr, Ni, Fe), which improved compositional stability and homogeneity. Prior to melting, the samples were subjected to vacuum and argon purging, and Ti was used as a sacrificial element to eliminate oxygen contamination. The alloy was remelted multiple times to ensure chemical uniformity. The resulting ingot was ground into 30–60 µm powders under an inert atmosphere to prevent oxidation.Structural and microstructural characterization were performed using XRD, SEM, TEM, and EDS analyses.Electrochemical measurements were conducted using a Swagelok cell with a three-electrode configuration in 6 M KOH electrolyte. The working electrode consisted of alloy powder mixed with Ni (3:1 ratio). Charge–discharge tests and EIS analysis were carried out to evaluate electrochemical performance. Hydrogen storage properties were investigated using a Sievert-type apparatus at temperatures between 25–300 °C over multiple hydrogenation/dehydrogenation cycles.

The $Mg_{0.5}Al_{12.5}Ni_{12.5}Fe_{12.5}Cr_{12.5}$ alloy exhibited a dominant BCC structure (~90.6 wt%) with a minor HCP phase, confirming successful Mg incorporation and improved homogeneity via lamination. TEM revealed nanoscale particles (5–20 nm), while SEM/EDS confirmed uniform composition without oxidation. The alloy delivered a maximum discharge capacity of 269 mAh/g, decreasing to 140 mAh/g after 50 cycles (51.85% retention), mainly due to surface degradation and $Mg(OH)_2$ formation, which limits hydrogen diffusion. EIS analysis showed that charge transfer resistance and hydrogen diffusion are the main limiting factors. Hydrogen storage reached 2.04 wt% at 300 °C with fast kinetics, while electrochemical results corresponded to ~1 wt%, indicating good consistency between methods.

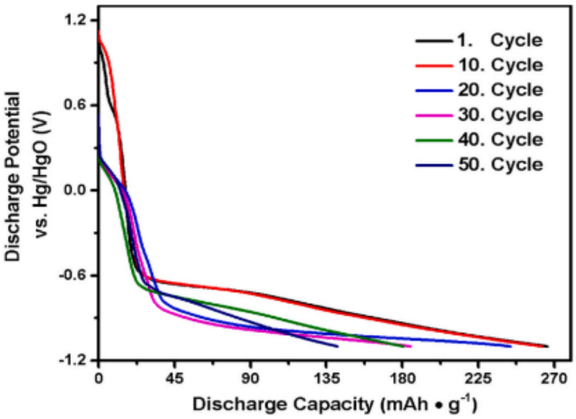

Figure 2. Discharge capacity as a function of cycle number for $Mg_{0.5}Al_{12.5}Ni_{12.5}Fe_{12.5}Cr_{12.5}$ alloy electrode at 273 K.

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Effect of mechanical alloying and activation on the diffusion behavior and durability of metal hydride bulk materials

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A serious issue in the way of widespread adoption of metal hydride hydrogen storage systems is the formation of ultrafine powders during their operation. Removing fine powder from the storage unit potentially causes fittings and valves clogging, degradation ("burning") of fuel cell membranes and the system failure. Accidental depressurization of the storage system can have serious consequence due to the high pyrophoricity of fine powders. Besides, dispersed powders have low thermal conductivity, which can lead to significant local overheating, sintering and thus cause swelling of the container. Along with that the processes of heat and mass transfer deteriorate dramatically. Therefore, the issue of preventing the formation of fine powders is extremely relevant and this study examines various approaches to its solution.

Mechanical activation (MA) in a high-energy ball mill with subsequent pressing [1-3] and laser beam powder bed fusion (LB-PBF) [4] as possible ways to prepare bulk metal hydride materials were considered.

It was found, that internal energy, high lattice defects concentration accumulated in MA powdersand their specific nanocrystalline state lead to the formation of contact bridges between material particles during pressing. As a result, the formed bulk material retains its integrity. It exhibits higher thermal conductivity and good durability in course of multiple hydrogen absorption-desorption cycles despite significant volumetric effects as it was demonstrated by dilatometric analysis (Fig. 1).

The LB-PBF technique is not convenient for the bulk sample preparation from hydrogen storage alloys for two reasons: 1) It involves a particle melting with subsequent crystallization. Therefore, the obtained specific nanocrystalline structure state of the particle is lost during processing; 2) LB-PBF technology requires the initial powder particle size of 30–80 µm. However, the average size of most hydrogen storage alloys (TiFe, $LaNi_5$, and Mg_2Ni) subjected to MA treatment is limited by the range from nano size up to about 5 µm. Therefore, the powder flow rate is dramatically decreased, and the bulk sample formation via LB-PBF becomes impossible.

We suggest that the fine nanocrystalline structure of powders is a key factor in the additive manufacturing of bulk porous samples from hydrogen storage alloys. The main idea is to keep a high density of microcrystalline defects inside these particles (large extent of grain and subgrain boundaries, large dislocation density, etc.), i.e., to keep large internal free volume that makes it possible to overcome the lattice volume change and to prevent destruction of the bulk samples during hydrogenation/dehydrogenation cycles.

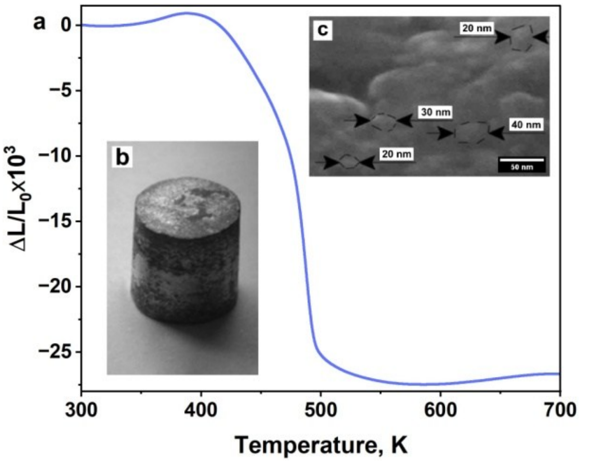

Figure 1. Dilatometric analysis of TiFe bulk hydrogenated samples: (a) change in length upon heating (hydrogen release from the sample); (b) general appearance of the sample after hydrogenation/dehydrogenation cycles; (c) SEM image of the bulk sample surface, obtained via MA with subsequent compacting (nanostructure of the sample).

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Acknowledgements

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The influence of the composition of Ni-P thin films on their electrocatalytic properties.

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The hydrogen evolution reaction (HER), a fundamental step in water electrolysis, is of critical importance as hydrogen fuel is considered a clean alternative to fossil fuels for the future. It is desirable that hydrogen be produced via carbon-free methods, utilizing only renewable energy and resources in the production process. The search for cost-effective and catalytically active electrocatalysts for HER remains at the forefront of challenges to its practical and widespread implementation. Transition metal-based compounds are among the primary and low-cost candidates for replacing platinum (Pt). Transition metal phosphides represent an important class of compounds formed by alloying metals with phosphorus. Among them, nickel phosphides (Ni_xP_y) stand out as cost-effective catalysts with unique properties and remarkable HER performance. They exhibit high stability under high current densities, which is particularly crucial for large-scale applications [1]. In Ni_xP_y compounds, metallic bonds (Ni-Ni) coexist with stronger ionic bonds-specifically, the bonding between nickel and phosphorus ions. These interactions impart Ni_xP_y with high thermal stability, hardness, and resistance to chemical degradation [2]. In the fabrication of electrocatalysts, phosphides are employed as effective additives that can enhance electrocatalytic performance by optimizing surface morphology and tuning the electronic structure [3]. The phase diagram of the system includes a wide range of nickel compounds with varying phosphorus content. In this study, Ni-P thin films were synthesized via electrolysis from two different electrolytes, and their electrocatalytic properties were subsequently investigated in an alkaline medium (1 M KOH). During the deposition from an electrolyte containing $NiCl_2 \cdot 6H_2O$, $Na_2HPO_4 \cdot 2H_2O$, $NaH_2PO_4 \cdot 2H_2O$ and H_3PO_4, X-ray phase analysis revealed the formation of the NiP_3 compound (sample 1). During the electrochemical deposition of Ni-P thin films from an electrolyte containing $NiCl_2 \cdot 6H_2O$, $NiSO_4 \cdot 6H_2O$, $NaH_2PO_4 \cdot 2H_2O$, and H_3PO_4, X-ray phase analysis revealed that the resulting film consisted of a mixture of two compounds: Ni_2P and NiP_2 (sample 2). Both samples were examined for their catalytic activity in the hydrogen evolution reaction (HER) under alkaline conditions. For this purpose, polarization curves were recorded in a 1 M KOH solution. The obtained experimental data are presented in the figure, which includes not only the two synthesized samples but also comparative curves of the catalytic activity of electrodes traditionally used in the HER. Based on these polarization curves, Tafel plots were constructed in the coordinates of E(V) - lgi.

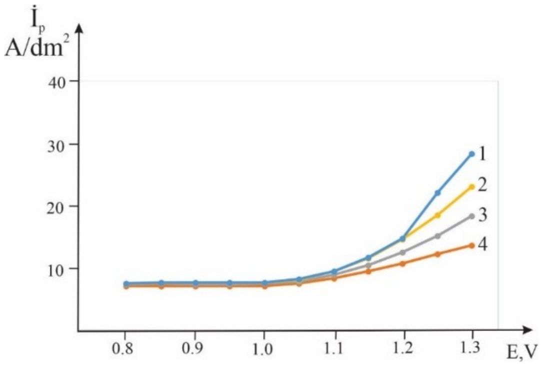

Figure 1. Electrocatalytic activity of the electrocatalysts in the HER in 1 M KOH:1 – Sample No. 1 (NiP_3), 2 – Sample No. 2 ($Ni_2P + NiP_2$), 3 – Steel-3, 4 – Nickel.

The slope of the Tafel plots was used to calculate the Tafel angles. The electrocatalytic activity of both samples exceeded that of pure nickel and steel, which are commonly used in industrial water electrolysis. It was found that, in an alkaline medium, the catalytic activity of sample 2, consisting of a mixture of two compounds, was lower and amounted to 203 mV/dec. The highest catalytic activity was observed for sample 1, with a Tafel slope of 135 mV/dec.

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The Role of Hydrogen in the HDH Process for Producing Titanium Alloy Powder for Additive Manufacturing

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The rapid development of additive manufacturing has increased the demand for high-quality and cost-effective metallic feedstock materials. Titanium alloys are widely used in AM due to their excellent mechanical properties, corrosion resistance, and biocompatibility.

This study investigates the hydriding–dehydriding (HDH) process as a sustainable approach for producing TiAl6Nb7 alloy powder from recycled materials. Hydrogen plays a crucial role by inducing temporary embrittlement through reversible binding, enabling efficient mechanical fragmentation. The HDH process can be applied to recycle titanium alloy waste no longer suitable for medical use. Hydrogenation increases material brittleness, allowing it to be mechanically crushed into powder by ball milling.

Hydration treatment, carried out under controlled parameters, aimed to increase brittleness. Using a planetary mill, hydrided TiAl6Nb7 alloy powder was obtained figure 1, featuring irregular particle shapes but favorable granulation, with a significant portion below 60 µm [1].

Figure 1. TiAl6Nb7 titanium powder after grinding of the hydrated sample [1]

Microstructural analysis of TiAl6Nb7 alloy produced by the HDH process was conducted at the Center for Advanced Materials (Sarajevo) using scanning electron microscopy (SEM) at the Faculty of Natural Sciences and Engineering, University of Ljubljana [2].

The results indicate that at HDH-produced TiAl6Nb7 powder represents a promising, cost-effective, and environmentally sustainable feedstock for additive manufacturing of biomedical and industrial components.

SEM and EDS analyses of hydrided TiAl6Nb7 alloy powder are shown in figures 2 and 3.

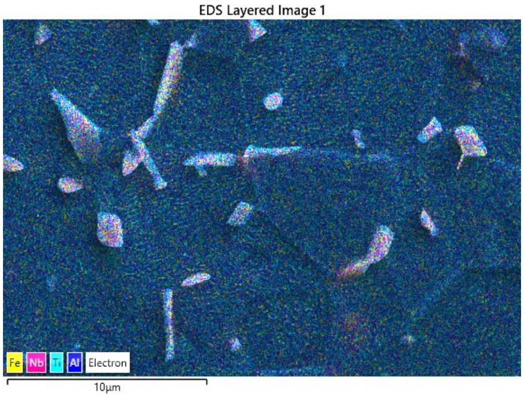

Figure 2. EDS representation of the primary phase of the matrix and the secondary phase [2]

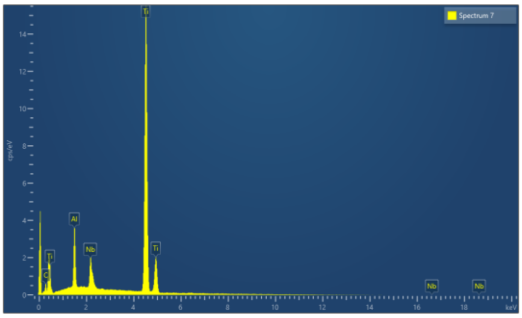

Figure 3. EDS spectrum of region from Figure 2 of hydrated alloy TiAl6Nb7 [1]

For the region which is shown in Figure 2 the average chemical contents of Al, Ti, and Nb is given in Table 1.

Table 1. Average chemical contents of Al, Ti, and Nb for region from Figure 2 for hydrated TiAl6Nb7 alloy powder, wt. %

	Al	**Ti**	**Nb**
Content wt. %	5.66	86.96	7.37

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Leading researcher for advanced materials in Center for advanced technologies in Sarajevo.
Reasearch activities: Structural properies improvement by high degree of plastic deformation, related to hydrogen storage of Mg alloys AZ31 and AZ91, in order to enable hydration and dehydration without turning into metal powder. Magnesium alloys as a medium for hydrogen storage in a bulk state. HDH (hydride-dehydride) process of recycling of titanium alloys, which is used to obtain titanium alloy powder with unchanged chemical composition.

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