FM 2: Energy Materials

Chair: Anna Grünebohm (Ruhr Universität Bochum, DE)

Time: Monday 9:30–11:30 Location: BEY/0138

FM 2.1 Mon 9:30 BEY/0138

Fundementals of elctrochemical hydrogen charging of MAX phases and their storage potential — •Rebeca Miyar, Adam C. Miles, Manoj Prabhakar, Lilian Vogl, Gerhard Dehm, Yug Joshi, Barak Ratzker, and Maria Jazmin Duarte — Max Planck institute for Sustainable Materials, Düsseldorf, Germany

Hydrogen storage remains a central challenge in the transition to renewable energy systems, as current technologies face limitations in scalability, safety, and efficiency. MAX phases, a class of nanolaminated carbides and nitrides composed of an early transition metal, an A-group element, and carbon or nitrogen, are perspective candidates for solid-state hydrogen storage due to their layered structure, which provides potential interstitial trapping sites. Although many theoretical studies discuss their hydrogen trapping behaviour, experimental evidence remains limited and previous work has focused only on gas-phase hydrogenation. Here, we present the first systematic study of electrochemical hydrogen charging and desorption in Ti2AlC and Ti3AlC2, which differ in their metal/ceramic layer ratio. Hydrogen trapping and release were analysed using thermal desorption spectroscopy, Kelvin probe measurements, and electrochemical methods. Two dominant trap types were identified in both materials, with their relative contributions reflecting the layer ratio. These results provide new insight into hydrogen permeation and trapping in MAX phases.

FM 2.2 Mon 9:45 BEY/0138

Multilayer Na intercalation in bilayer graphene — •Mahdi Ghorbani-Asl and Arkady V. Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany.

The intercalation of atomic and molecular species into layered materials has emerged as a powerful route for creating novel encapsulated two-dimensional systems with tunable physical properties. Among these, alkali-metal intercalation in graphitic carbon has been widely explored for energy-storage applications. However, sodium (Na) intercalation into bulk graphite is predicted to be energetically unfavorable, making it particularly challenging to realize experimentally. In this work, we combine first-principles calculations with scanning transmission electron microscopy (STEM) to investigate Na intercalation into bilayer graphene. Using DFT simulations, we analyze the energetics and atomic structures of Na intercalants in single-layer and multilayer configurations, and evaluate how charge transfer between graphene and the Na atoms affects their stability. Our simulations reveal that the lowest-energy structure is an fcc trilayer with an A-B-C stacking sequence, whose projected atomic arrangement is fully consistent with the STEM observations. These findings provide new insight into Na intercalation mechanisms and may support the development of future sodium-ion battery technologies.

FM 2.3 Mon 10:00 BEY/0138

The Role of Lone Pairs in Fast Oxide Ion Conduction in $Bi_{0.8}Pr_{0.2}O_{1.5}$ — •Marcin Kryński — Warsaw University of Technology

Elucidating the microscopic processes that enable rapid oxide-ion transport is key to advancing solid electrolyte design. In this study, we integrate total neutron scattering with reverse Monte Carlo modelling and ab initio molecular dynamics to dissect the structural and electronic mechanisms underlying a pronounced conductivity increase observed across the order/disorder phase transition. Our results reveal that this transition is driven not by changes in the cation framework, but by a collective reorganization of oxide ions and local coordination environments. Specifically, oxide ions shift from the edges of fluorite-like blocks into the van der Waals gap, where they gain access to extended, predominantly two-dimensional diffusion pathways. Concurrently, BiO_4 units undergo a subtle yet systematic reorientation linked to the stereochemical activity of Bi^{3+} lone pairs. Although the local coordination of Bi remains largely preserved, the orientation of these lone pairs evolves in tandem with the redistribution of oxide ions, suggesting a dynamic coupling reminiscent of a paddle-wheel-type mechanism. This interplay between lone-pair-driven asymmetry and anion mobility provides a unified mechanistic picture of how structural flexibility and electronic degrees of freedom cooperate to enhance high-temperature oxide-ion transport. The insights gained here establish general principles for designing fast-ion conductors in systems where active lone pairs play an essential role.

Coffee break

FM 2.4 Mon 10:30 BEY/0138

Metal Poisoning of Nafion Proton Exchange Membrane — •Souvik Mitra[1], Jialiang Liu[1], Kristina Fröhlich[1], Simone Köcher[1,2], Christoph Scheurer[2,1], and Rüdiger-A. Eichel[1] — [1]IET-1, Forschungszentrum Jülich GmbH, 52425 Jülich, DE — [2]Fritz-Haber-Institute der MPG, 14195 Berlin, DE

Metal-ion contamination of Nafion proton-exchange membranes (PEMs) remains a persistent durability and performance issue in PEM fuel cells. Metal cations originating from insufficiently deionized feed water, coolant leaks, or corrosion of metallic cell components can exchange with protons at the sulfonate groups (SO_3^-) of Nafion, thereby reducing proton conductivity and overall cell performance.
In this work, we combine atomistic molecular dynamics simulations with in-plane conductivity measurements to build a consistent picture of how a broad series of mono-, di-, and trivalent cations affect transport in Nafion under comparable conditions. For monovalent ions (Li^+, Na^+, and K^+), our study reveals a reversal of the familiar mobility trend of these cations in the presence of Nafion membrane compared to bulk water, reflecting the competition between ion hydration and specific binding to the SO_3^- groups of Nafion. Our study also shows that, as cation charge increases from +1 to +2 to +3, their mobility drops significantly, correlating with longer residence times at sulfonate sites and increasingly multidentate SO_3^- coordination.
Our study highlights the strengths of simulations in elucidating the atomistic origin of diffusivity trends, but also their challenges in making reasonable physical approximations.

FM 2.5 Mon 10:45 BEY/0138

Synchrotron X-ray Characterization of Irradiated Ag/PVA Polymer Electrolyte — Mohamed Salah Soliman Asser and •Mohamed Salah Soliman Asser — Polymer Chemistry Department, National Center for Radiation Research and Technology, Egyptian Atomic Energy Authority, Cairo, Egypt.

Polymer electrolyte membrane thin films were developed and characterized for potential use in electroconductive applications. Polymer composites of polyvinyl alcohol (PVA), sulfuric acid, ethanol, and silver nitrate were prepared using both casting and dip-coating techniques. For the dip-coating method, glass slides were first cleaned by immersion in acetone, rinsed with isopropanol, and dried. The prepared polymer composite solutions were then dip-coated onto the glass substrates. The coated slides were irradiated at three doses: 62 J/cm2 (low), 251 J/cm2 (medium), and 502 J/cm2 (high) using the DXRL beamline. High-resolution X-ray diffraction (HR-XRD) analyses were performed at the Elettra Synchrotron Laboratory, Trieste, Italy, using the MCX beamline at a glancing angle of 1°. The X-rays had an energy of 12 keV (λ = 1.033 Å). Diffraction patterns were recorded in the 2θ range of 1*80° with a step size of 0.01° and an exposure time of 1 s per step for the Ag*PVA samples.

FM 2.6 Mon 11:00 BEY/0138

Tailoring Electrochemical Functionality of Transition-Metal Glycerolates for Next-Generation Energy Storage Devices — •Ali Hyder[1,2], Irlan S Lima[2], Zahid ullah Khan[2], Ayaz Ali Memon[1], and Lucio Angnes[2] — [1]National Centre of Excellence in Analytical Chemistry, University of Sindh, Jamshoro 76080, Pakistan — [2]Departament de Química Fundamental, Institute de Química, University of São Paulo, Av. Prof. Lineu Prestes, 748 * 05508-000, São Paulo, SP, Brazil

Abstract Metal glycerolates are emerging as promising precursors and active materials for electrochemical energy-storage systems due to their tunable coordination chemistry, oxygen-rich structures, and flexible architectures. In this study, transition-metal glycerolates (Mn, Co, Ni, Cu, Fe) were synthesized via a controlled solvothermal method to ex-

plore how formation and nanoscale morphology influence electrochemical performance. Structural analyses show that the resulting M*O*C networks form layered or clustered architectures that enhance ion diffusion and electron transport. Used as electrode materials either directly mild thermal treatment the glycerolates exhibit strong pseudo capacitance, improved redox kinetics, and good stability. Metal glycerolytes deliver the highest capacitance due to synergistic redox activity and accessible surfaces. Overall, the results demonstrate the potential of metal glycerolates as low-cost, versatile candidates for advance hybrid energy-storage devices.

FM 2.7 Mon 11:15 BEY/0138

Thermoelectric properties of In-doped Bi2Te3 crystalline bulk alloys — •Alaa Adam[1] and E. Ibrahim[2] — [1]Sohag University — [2]Sohag university

Influence of indium doping on the structure, morphology and thermoelectric properties of bulk Bi2Te3 is investigated in the current work. Bi2Te3 and Bi2-xInxTe3 crystalline bulk samples have been fabricated using a simple mono-temperature melting method. Analyses employing X-ray diffraction (XRD) and scanning electron microscopy (SEM) techniques proved the existence of the concerned phases. In addition, morphology and internal structure have been examined via the scanning electron microscopes and the energy dispersive X-ray (EDX) spectroscopy. Thermoelectric properties were determined in a temperature range between 300*700 K. The electrical conductivity (σ) against the temperature showed metallic-like behavior. Carrier concentration has increased with in-doping. The Seebeck coefficients (S) of the synthesized alloys proved the domination of n-type conduction due to consistently negative S values. The largest Seebeck coefficient was recorded at 203.5 *V/ K which was observed at 700 K for the pristine Bi2Te3 sample. The highest power factor was found at PF = 5.46 mWm-1K-2, obtained for Bi2Te3 at room temperature. Thermal conductivity was measured and studied against temperature elevation. It was found that the thermal conductivity of the In-doped Bi1.98In0.02Te3 alloys are significantly reduced compared with that of the pure Bi2Te3 material.