

## KFM 19: Materials for Energy Storage II (joint session KFM/ CPP)

Organizer: Martin Diestelhorst - Martin-Luther-Universität Halle-Wittenberg - Halle

Time: Wednesday 15:00–17:50

Location: EMH 025

Invited Talk KFM 19.1 Wed 15:00 EMH 025

**Electrical double layer capacitors, Insights from fundamental research and their impact on storage devices** — ●GUDRUN REICHENAUER — Bavarian Center for Applied Energy Research, 97074 Würzburg, Germany

Electrical double layer capacitors (EDLC) are important components in the toolbox of currently available electrical storage devices, serving in particular applications that require reliability and high power density, such as e.g. emergency doors in airplanes, or high cycling stability at low to medium energy density, such as electrically driven buses for public transportation. Typically, optimization of EDLCs is performed by empirical tests of different active materials, binders and conductive additives. However, only limited systematic studies are available to address questions, such as

What are the optimized structures in terms of pore sizes and porosity of the active component?

How do the micropore (pores < 2 nm) characteristics affect the storage in the presence of organic, aqueous and polymer electrolytes?

What is the impact of the device layout vs. the properties of the electrode itself on the performance (energy and power density) of an EDLC?

The talk will address some of these questions using model carbon materials that allow systematic variation of key parameters and also show how new in-situ/in-operando techniques can further support a more targeted development of EDLC storage devices for different types of applications.

KFM 19.2 Wed 15:30 EMH 025

**Pyrolytic graphite electrodes intercalated by  $\text{AlCl}_4$  anions probed by X-ray tomography and small angle X-ray scattering** — ●GIORGIA GRECO<sup>1</sup>, GIUSEPPE ELIA<sup>2</sup>, DRAGOMIR TACHEV<sup>3</sup>, ARMIN HOELL<sup>1</sup>, ROBERT HAHN<sup>4</sup>, and SIMONE RAOUX<sup>1,5</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany — <sup>2</sup>Technische Universität Berlin, Research Center of Microperipheral Technologies, Gustav-Meyer-Allee 25, 13355 Berlin, Germany — <sup>3</sup>Institute of Physical Chemistry, Bulgaria Academy of Science, Acsd. G. Bonchev Str. Bl.11, 1113 Sofia, Bulgaria — <sup>4</sup>Fraunhofer-Institut für Zuverlässigkeit und Mikrointegration, Gustav-Meyer-Allee 25, 13355 Berlin, Germany — <sup>5</sup>Department of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Due to the cost and limited resources of lithium, the use of Li-ion batteries for large scale applications is nowadays under discussion. Aluminum based secondary batteries could be a viable alternative to the present Li-ion technology because of their high volumetric capacity. Additionally, the low cost aluminum makes these devices appealing for large-scale electrical energy storage. We report the structural characterization by a combination of x-ray tomography and SAXS (Small Angle X-ray Scattering) related to electrochemical performances of aluminum tetrachloride electrolyte in an aluminum/graphite battery. The aim of this work is to characterize the micro- and nano-structure of highly ordered graphite during the electrochemically induced reaction mechanism of  $\text{AlCl}_4$  intercalation.

KFM 19.3 Wed 15:50 EMH 025

**Structural and microstructural evolution during oxygen intercalation in  $\text{Pr}_2\text{NiO}_{4.25}$  single crystal investigated by in-situ synchrotron diffraction** — ●AVISHEK MAITY<sup>1,2</sup>, RAJESH DUTTA<sup>3</sup>, MONICA CERETTI<sup>3</sup>, DMITRY CHERNYSHOV<sup>4</sup>, and WERNER PAULUS<sup>3</sup> — <sup>1</sup>Institut für Physikalische Chemie, Georg-August Universität Göttingen, 37077 Göttingen, Germany — <sup>2</sup>Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching, Germany — <sup>3</sup>Institut Charles Gerhardt, Université de Montpellier, 34095 Montpellier, France — <sup>4</sup>The European Synchrotron-ESRF, 38000 Grenoble, France

$\text{Pr}_2\text{NiO}_{4+x}$  is a promising oxygen membrane material having excellent ionic conductivity at moderate T. Oxygen diffusion occurs through interstitial sites via phonon assisted diffusion mechanism. We found  $\text{Pr}_2\text{NiO}_{4.25}$  to be structurally extremely complex, showing large oxygen (interstitial) and charge ( $\text{Ni}^{2+}/\text{Ni}^{3+}$ ) ordered domains, and forming giant unit cells up to  $6000000 \text{ \AA}^3$ . In order to explore the oxy-

gen diffusion from structural and microstructural aspect as a function of oxygen stoichiometry ( $0 < x < 0.25$ ), we investigated in-situ electrochemical (EC) oxygen intercalation on a 50 micron highly twinned single crystal mounted in a specially designed EC cell using synchrotron diffraction at BM01A@ESRF. We have followed phase transitions (ortho  $\rightarrow$  tetra  $\rightarrow$  ortho) and evolution of domain structure with a very special focus on the presence or absence of grain boundaries. This in-situ study allowed during an EC reaction to explore whole reciprocal space i.e. microstructure, twin domains including diffuse scattering.

KFM 19.4 Wed 16:10 EMH 025

**A green magnetic cooling device built using upcycled NdFeB magnets** — ●DIMITRI BENKE<sup>1</sup>, JONAS WORTMANN<sup>1</sup>, MARC PABST<sup>1</sup>, TINO GOTTSCHALL<sup>2</sup>, ILIYA RADULOV<sup>1</sup>, KONSTANTIN SKOKOV<sup>1</sup>, OLIVER GUTFLEISCH<sup>1</sup>, DAVIDE PROSPERI<sup>3</sup>, PETER AFIUNY<sup>3</sup>, and MIHA ZAKOTNIK<sup>3</sup> — <sup>1</sup>TU Darmstadt, Darmstadt, Deutschland — <sup>2</sup>Helmholtz-Zentrum Dresden-Rossendorf, Rossendorf, Deutschland — <sup>3</sup>Urban Mining Company, Austin, USA

Magnetocaloric devices hold the potential to satisfy the rising demand for cooling in the future. One remaining challenge is to reduce the high ecological footprint of the permanent magnets driving the magnetic cooling cycle. Existing devices use neodymium-iron-boron (NdFeB)-type permanent magnets, which account for more than 50% of the ecological footprint of the appliance. To overcome this hurdle, TU Darmstadt and Urban Mining Company have built the first working magnetocaloric device that uses recycled NdFeB as a magnetic field source. Coupling this with optimisation of the magnets and their geometry, it is possible to further reduce the ecological footprint. Together, these two approaches help to position magnetic cooling as a realistic and sustainable cooling technology.

20 min. break

KFM 19.5 Wed 16:50 EMH 025

**Electromagnetic Functionalization of Wide Band Gap Dielectric Oxides by Interstitial Doping** — ●DAE-SUNG PARK<sup>1,3</sup>, HAIYUAN WANG<sup>2</sup>, DIANA RATA<sup>3</sup>, AKASH BHATNAGAR<sup>1,3</sup>, IGOR MAZNICHENKO<sup>3</sup>, SERGEY OSTANIN<sup>3</sup>, and KATHRIN DÖRR<sup>3</sup> — <sup>1</sup>Zentrum für Innovationskompetenz SiLi-nano, Halle, Germany — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — <sup>3</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

In solid-state oxides, methods such as chemical doping/alloying, mechanical strain, defect engineering, and integration of distinct materials, have been conventionally used to modify a wide range of physical and chemical properties. Here, we demonstrate an extraordinary interstitial doping effect centred around a light element (boron) cation. The host matrix is a novel composite system synthesised from discrete bulk  $\text{LaAlO}_3:\text{LaBO}_3$  compounds. Our results show a spontaneous ordering of the interstitial boron cations within the host  $\text{LaAlO}_3$  lattices, and subsequent effective spin-polarized charge injection into the neighbouring cations. These ordered interstitials lead to a series of remarkable functional properties, namely, cation-dominated electrical switching and ferromagnetism. Therefore, interstitial boron doping serves to transform a wide band gap and non-magnetic dielectric bulk oxide into a high-temperature ferromagnetic ionic-electronic conductor. This interstitial doping effect is proposed to be a general route for tailoring new multifunctional properties in bulk oxides for smart materials applications such as non-volatile information and spintronic devices.

KFM 19.6 Wed 17:10 EMH 025

**The impact of different Si surface terminations in the (001) n-Si/NiOx heterojunction on the oxygen evolution reaction (OER) by XPS and electrochemical methods** — ●SVEN TENGELER, MATHIAS FINGERLE, WOLFRAM CALVET, CÉLINE STEINERT, BERNHARD KAISER, THOMAS MAYER, and WOLFRAM JAEGERMANN — Technische Universität Darmstadt

The interaction between (001) n-Si and NiOx was investigated with regard to the oxygen evolution reaction (OER), applicable either for

water splitting or CO<sub>2</sub> reduction. Thin layers of NiO<sub>x</sub> were deposited step by step by reactive sputter deposition and analyzed in-situ after each step using X-ray photoelectron spectroscopy (XPS) for Si with different surface preparations: H-termination, thermally grown oxide (2 Å) and native oxide (4 Å). Upon contact formation the initial flat band like situation in the Si substrates changed to a 0.35-0.4 eV upward band bending for all three heterojunctions, hole extraction barriers are low.

The observed similarities in the heterojunctions should result in the same similarities for the OER performance. However, cyclic voltammetry measurements reveal a shift of more than 0,2 V in dependence of the surface treatment. Using chopped light measurements, this under-performance could be attributed to a higher density of defect states at the Si surface. Apparently a 4 Å SiO<sub>2</sub> layer is sufficient protection to prevent the formation of defect states during NiO<sub>x</sub> deposition, thinner protective layers or none at all result in increased defect states, while thicker layers perform poorly due to their high ohmic resistance.

KFM 19.7 Wed 17:30 EMH 025

**Interaction of water with wet-chemically etched p-GaInP<sub>2</sub>(100) surface** — ANDREAS HAJDUK<sup>1</sup>, ●MIKHAIL LEBEDEV<sup>2</sup>, BERNHARD KAISER<sup>1</sup>, and WOLFRAM JAEGERMANN<sup>1</sup> — <sup>1</sup>TU Darm-

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Photoelectrochemical water splitting offers the possibility to convert solar energy directly into a chemical fuel and therefore is a promising candidate for a sustainable energy solution in the future. GaInP<sub>2</sub> with a direct bandgap of 1.8-1.9 eV shows so far the highest reported solar-to-hydrogen conversion efficiencies. Nevertheless, the fast photo-corrosion of III-V semiconductors in aqueous solution presents a major obstacle for their use as efficient and stable photoelectrodes. Interaction of water with chemically etched p-GaInP<sub>2</sub>(100) surface covered with a submonolayer of residual oxides is studied by synchrotron photoemission spectroscopy to gain insight into the solid/solvent interaction at the semiconductor/electrolyte interface. Photoemission spectra obtained after emersion of the semiconductor from liquid water at room temperature and adsorption of H<sub>2</sub>O molecules at liquid-nitrogen temperature are compared to understand the chemistry of the GaInP<sub>2</sub>(100)/H<sub>2</sub>O interface. Valence band spectra indicate dissociative adsorption of water molecules both after emersion and after adsorption experiments. Surface-sensitive core level spectra reveal the interaction of H<sub>2</sub>O molecules with surface phosphorous and gallium atoms.