KFM 12: Materials for Energy Storage (joint session KFM/CPP)

Time: Thursday 9:30–11:50   Location: HSZ 301

KFM 12.1   Thu 9:30   HSZ 301

Investigation of Li diffusion mechanisms in V_2O_5 — •Fabian Dietrich and Eduardo Cisternas Jara — Núcleo Milenio Multi-Mat & Departamento de Ciencias Físicas, Universidad de La Frontera, Temuco, Chile

Vanadium pentoxide (V_2O_5) is a promising candidate for the use as cathode material in lithium ion batteries (LiB) due to its layered structure. For the use as electrode material, it is necessary to understand fundamental aspects of its structure as well as mechanisms during the charging and discharging process. Hence, we investigate the diffusion of lithium ions in that material, paying attention to vanadium pentoxide species with different amount of inserted lithium.

The investigations are done by simulation of the processes using density functional theory (DFT) in the periodic boundary condition, also in combination with plane-wave basis sets and dispersion correction. Diffusion pathways are calculated using the nudged-elastic band (NEB) method. Resulting barrier heights are used for subsequent Monte-Carlo simulations. Frequency calculations are used to estimate the diffusion coefficients, which are also used in the MC simulations.

We assumed different diffusion mechanisms for the pure V_2O_5 and the lithiated species LiV_2O_5. While in V_2O_5 a quite free diffusion of Li ions is possible, the occupation of distinct lattice positions by Li ions leads to a blocking of certain pathways. Thus, the knock-off mechanism is proposed for LiV_2O_5. This assumption could be confirmed by the calculations, comparing different mechanisms for the diffusion in LiV_2O_5.

KFM 12.2   Thu 9:50   HSZ 301

Evaluation of the Applicability of the Brick Layer Model for Describing the Electrical Transport within Ceramic Materials — •Janis K. Eckhardt[1,2], Markus S. Friedrich[2,3], Matthias T. Elm[2,3,4], Peter J. Klar[2,3], and Christian Heiliger[1,2] — [1]Institute for Theoretical Physics, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Center for Materials Research (LaMa), Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [3]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [4]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Gießen, Germany

In literature, the transport properties of ceramics such as the active cathode material within lithium ion batteries are commonly described by making use of the so called Brick Layer Model (BLM). The BLM cannot account for percolation effects. However, the microstructure of real devices, e.g. secondary materials of cathodes or thin films is such that disorder will lead to percolation effects. In order to account for these effects and to validate the applicability of the BLM an impedance network model based on Kirchhoff's current law has been developed. With its help it is possible to compute impedance spectra and current density distributions of defined or random structures that mimic the properties of the real microstructure. Comparing the computational result to the prediction of the BLM, it becomes obvious that an additional semicircle(s) and signal(s) respectively in the impedance and distribution of relaxation times spectra may occur. This effect can be attributed to the multidimensional transport mechanism within the structures which is not accounted for in the commonly used BLM.

KFM 12.3   Thu 10:10   HSZ 301

First principles calculation on intrinsic defects properties of Sodium Niobate — •Lorenzo Villa — Fachgebiet Materialmodellierung, Institut für Materialwissenschaft, TU Darmstadt, Otto-Berndt-Straße 3, D-64287 Darmstadt, Germany

In recent years extended research has been focusing on improving the properties of capacitors for energy storage applications. In this context, lead-free antiferroelectric materials (AFE) are excellent candidates due to their ability of displaying high energy density, high energy efficiency and low environmental impact. In this class of compounds, $NaNbO_3$ (NN) is amongst the most promising materials, due to the possibility to obtain double P-E loops at room temperature. One of the mostly used methods to obtain narrower antiferroelectric P-E loops is via doping. Intrinsic defects can interact with the dopants and therefore can have an impact on AFE properties. In order to investigate the interaction of intrinsic defects with dopants, we have studied the contribution of vacancies to intrinsic electron and hole conductivity and their interaction with different types of dopants (Sr, Ca, Mn). All calculations

were performed in the framework of Density Functional Theory using Hybrid functionals. In particular, we have investigated the formation energies of all vacancy types considering all possible charge states in five different regions of the stability diagram.

20 min. break

KFM 12.4   Thu 10:50   HSZ 301

Glass ceramics with proton conducting crystalline phases — •Laura Weisshoff[1,2], Martin Letz[1,2], Martin Jourdan[1], and Martun Hovhannisyan[2] — [1]Johannes Gutenberg Universität Mainz — [2]Schott AG Mainz

Proton conducting crystal phases such as the perovskite type have their application in proton conducting fuel cells (PCFC), sensors and hydrogen separation. A reduction of the operating temperature due to highly efficient inorganic proton conducting materials is an important development target. For this, a proton-conducting electrolyte is a key component and an optimized material is required. Standard ceramic solutions show high sintering temperature and pores. A non-gas tight material can lead to a catastrophic failure of the PCFC. Therefore, we develop pore free glass ceramics with lower sintering temperature. The present talk reports the progress of glass ceramics with proton conducting crystalline phases.

KFM 12.5   Thu 11:10   HSZ 301

Rapid, clean and scalable synthesis of microporous functional MOFs and their non-conventional forms via mechanochemistry — •Krunoslav Užarević — Ruder Boskovic Institute, 10000 Zagreb, Croatia

Here we present the application of mechanochemical reactions,[1] i.e. reactions between solid reactants induced by mechanical force, for a rapid, green and room-temperature transformation of environmentally safe metal precursors, oxides or hydroxides into most relevant microporous MOFs, such as HKUST-1, MOF-74[5] or zirconium-based MOFs of UiO[3] and NU- families, and also their multi-metal or amorphous derivatives not accessible from solution. We show here how the milling produces high-quality MOFs quantitatively in multigram quantities by using only a catalytic amount of *green liquids, such as methanol or water.

In situ synchrotron X-ray powder diffraction monitoring[8] revealed that the mechanochemical formation of MOFs often proceeds through intermediate phases, most of which are inaccessible from solution procedures. It is possible to isolate and characterize these intermediates, and also use them for the controllable synthesis of multi-metal MOFs, such as various bimetal MOF-74 materials, with interesting magnetic properties and strong potential for new catalytic reactivity.

[3] James et al, Chem. Soc. Rev. 2012, 42, 7638. [2] Julien et al, J. Am. Chem. Soc., 2016, 138, 2929. [3] Užarević et al., Chem. Commun. 2016, 52, 2133. [8] a) Užarević et al., J. Phys. Chem. Lett, 2015, 6, 4129.

KFM 12.6   Thu 11:30   HSZ 301

Actuation and electrostriction of composite films with heterogenous filler clustering — •Elshad Allahyarov — Duisburg-Essen University, Theoretical Chemistry

Controlled actuation of electroactive polymers with embedded high dielectric nanoparticles is theoretically analyzed. If the inclusions are placed randomly in the elastomer body, the composite always contracts along the direction of the applied field. For a simple cubic distribution of inclusions, contraction occurs if the applied field is directed along the [001] direction of the lattice. For inclusions occupying the sites of other lattice structures such as body-centered or face-centered cubic crystals, the composite elongates along the field direction if it is applied along the [001] direction. The stability of the elongation against the imperfectness of the lattice site positions and the distortion ratio of the initial structures are examined. Finite elongation windows show up for the initially distorted body-centered cubic and face-centered cubic crystals as a function of the distortion ratio of the initial structure. The existence of these elongation windows are also predicted from the analysis of the electrostatic energy of the distorted body-centered cubic and face-centered cubic lattice structures. Our results indicate that the electrostriction effect, which is the main contribution to the actua-

tion of low aspect-ratio composites, strongly depends on the geometry of the spatial distribution of nanoparticles, and can thereby largely be tuned.