

## MM 42: Materials for Energy Storage and Conversion - Functional Materials

Time: Wednesday 15:45–17:00

Location: IFW D

MM 42.1 Wed 15:45 IFW D

**Charge carrier diffusion in MgSc<sub>2</sub>Se<sub>4</sub> spinel structures** — ●MANUEL DILLENZ, MOHSEN SOTOUDEH, and AXEL GROSS — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

New battery technologies have to meet a multitude of requirements in order to compete with Li-ion batteries, among them a sufficiently high ionic mobility both in the electrolyte and the electrodes. Materials that crystallize in the spinel structure represent promising materials that could meet this requirement. Here we present first-principles electronic structure calculations based on density functional theory (DFT) that have been performed to study the charge carrier diffusion in the MgSc<sub>2</sub>Se<sub>4</sub> spinel structure. MgSc<sub>2</sub>Se<sub>4</sub> exhibits very low diffusion barriers for Mg ion diffusion and is therefore a good candidate for solid electrolytes in Mg-ion batteries. In order to elucidate the factors determining the ion mobility we have also determined the diffusion barriers of other mono- and bivalent ions in this material and various other spinel structures in order to be able to derive chemical trends. These calculations show that the size and the charge of the ions influence the ion mobility. We will discuss further factors that could affect the ion mobility.

MM 42.2 Wed 16:00 IFW D

**Defect Calculations to Explain Charge-Carrier Transition in Disordered Chalcogenides** — ●VALENTIN EVANG<sup>1</sup>, JOHANNES REINDL<sup>2</sup>, ALEXANDER ROCHOTZKI<sup>2</sup>, MATTHIAS WUTTIG<sup>2,3</sup>, and RICCARDO MAZZARELLO<sup>1,3</sup> — <sup>1</sup>Institute for Theoretical Solid State Physics, RWTH Aachen University, 52056 Aachen — <sup>2</sup>I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen — <sup>3</sup>JARA-FIT, RWTH Aachen University, 52056 Aachen

Phase-change materials (PCMs) like GeSbTe and other chalcogenides promise to be key ingredients for future non-volatile memory thanks to their remarkable dynamic properties when switched between their crystalline and amorphous phases. Furthermore, they show features in atomic bonding, recently coined meta-valent, that are incompatible with the well-known bonding types and could play an important role in the design of materials with specific phase-change properties.

For a related material, the disordered cubic phase of PbSbTe, experiments reveal a transition from n-type to p-type conduction as a response to annealing at high temperatures. During this process, only subtle changes in the crystal structure take place, pointing towards varying types of self-doping to cause the transition.

Here, we employ density functional theory to compute the formation energies of various possible defects in the disordered cubic and related phases of PbSbTe. It is found that, upon reducing the disorder on the lattice, the most favorable defect type changes in accordance with the observed n-to-p charge-carrier transition, representing a mechanism to tailor transport properties in PCMs by their level of disorder.

MM 42.3 Wed 16:15 IFW D

**Understanding the charge trapping-detrapping in undoped- and carbon doped GaN** — ●SUCHINDER SHARMA<sup>1,2</sup>, FRIEDERIKE ZIMMERMANN<sup>1</sup>, JAN BEYER<sup>1</sup>, EBERHARD RICHTER<sup>3</sup>, and JOHANNES HEITMANN<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, Technical University Bergakademie Freiberg, 09599 Freiberg, Germany — <sup>2</sup>Helmholtz-Zentrum Dresden-Rossendorf, Helmholtz-Institute Freiberg for Resource Technology, 09599 Freiberg, Germany — <sup>3</sup>Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, 12489 Berlin, Germany

In the present contribution, we present our results on the thermoluminescence (TL) experiments on the GaN samples prepared by HVPE

method, to understand the charge trapping-detrapping dynamics in the temperature range, 273–650 K. Interestingly, the undoped GaN sample showed a persistent luminescence (PersL) emission upon band-to-band and localized excitations (blue, green and red), which lasts for more than 9 h. Upon carbon doping, the PersL is quenched significantly, suggesting, that the population of defects responsible for the room temperature trapping-detrapping decreases with an increase in the carbon doping. Further, for low carbon containing sample, a new deep defect around 530 K is observed. The population of this defect further decreases for high carbon containing samples.

MM 42.4 Wed 16:30 IFW D

**Electronic structure and core electron fingerprints of caesium-based antimonides for ultra-bright electron sources** — CATERINA COCCHI<sup>1,2</sup>, SONAL MISTRY<sup>3</sup>, MARTIN SCHMEISSER<sup>3</sup>, ●RAYMOND AMADOR<sup>1,2</sup>, JULIUS KUEHN<sup>3</sup>, and THORSTEN KAMPS<sup>1,3</sup> — <sup>1</sup>Humboldt-Universität zu Berlin, Institut für Physik, 12489 Berlin, DE — <sup>2</sup>Humboldt-Universität zu Berlin, IRIS Adlershof, 12489 Berlin, DE — <sup>3</sup>Helmholtz-Zentrum Berlin, 12489 Berlin, DE

The development of novel photocathode materials for ultra-bright electron sources demands understanding of intrinsic material properties, given constraints of growth and operational conditions. In a joint *ab initio* and experimental work, we propose a method to relate computed and measured core-level shifts and quantum efficiency of three alkali antimonides, which are particularly appealing for their absorption in the visible region. In our density-functional theory calculations we focus on Cs<sub>3</sub>Sb, Cs<sub>2</sub>KSb, and CsK<sub>2</sub>Sb. Experimentally, Cs-K-Sb samples with different stoichiometries and relative elemental content are investigated using x-ray photoemission spectroscopy (XPS). The largest core-level shifts (2 eV and 0.5 eV for K 2*p* and Sb 3*d*, respectively) can be correlated to XPS survey spectra, where such peaks are clearly visible. Core-level shifts can thus be used to identify specific compositions of Cs-K-Sb materials and their relation to measured values of quantum efficiency. Our results represent the first step towards a robust connection between the experimental preparation and characterisation of photocathodes, the *ab initio* prediction of their electronic structure, and the modeling of emission and beam formation processes.

MM 42.5 Wed 16:45 IFW D

**The effect of crystallinity of layered transition metal disulfide on the performance of potassium-ion batteries: The case of molybdenum disulfide** — ●YULIAN DONG, HUAPING ZHAO, and YONG LEI — Institut für Physik & IMN MacroNano\* (ZIK), Technische Universität Ilmenau, Ilmenau, Germany

Layer-structured transition metal dichalcogenides (LS-TMDs) are being studied in potassium-ion batteries owing to their structural uniqueness and electrochemical mechanisms. In this work, the dependence of electrochemical performance on the crystallinity of LS-TMDs has been investigated. Taking MoS<sub>2</sub> as an example, lower crystallinity can alleviate diffusional limitation in 0.5\*3.0 V, where intercalation reaction takes charge in storing K-ions. Higher crystallinity can ensure the structural stability of the MoS<sub>2</sub> layers and promote surface charge storage in 0.01\*3.0 V, where conversion reaction mainly contributes. The low-crystallized MoS<sub>2</sub> exhibits an intercalation capacity (118 mAh/g) and great rate capability (41 mAh/g at 2 A/g), and the high-crystallized MoS<sub>2</sub> delivers a high capacity of 330 mAh/g at 1 A/g and retains 161 mAh/g at 20 A/g. It shows that when intercalation and conversion reactions both contribute to store K-ions, higher crystallinity ensures the structural stability of the exfoliated MoS<sub>2</sub> basal layers and promotes surface-controlled charge storage.