

## KFM 2: Materials for Energy Storage

Chairman: Theo Scherer (KIT Karlsruhe)

Time: Tuesday 11:15–11:45

Location: H5

KFM 2.1 Tue 11:15 H5

**Self-assembled monolayers of *para*-aminobenzoic acid on  $V_2O_5$  - a theoretical and experimental study** — •FABIAN DIETRICH<sup>1</sup>, JUAN FERNANDEZ<sup>2</sup>, EDUARDO CISTERNAS<sup>1</sup>, and MARCOS FLORES<sup>2</sup> — <sup>1</sup>Universidad de La Frontera, Temuco, Chile — <sup>2</sup>Universidad de Chile, Santiago, Chile

Lithium ion batteries (LIB) can contribute to environment-friendly energy supply due to the storage for renewable energies. As important part of their characteristics, the number of charge/discharge cycles and the capacity after several cycling processes strongly depend on the electro-chemical reactions taking place on the surface of the electrodes, *e.g.* building the so called solid-electrolyte interface (SEI). To control the formation of the SEI, the surface can be functionalized with organic molecules, building a self-assembled monolayer (SAM).

We investigated the assembling of *para*-aminobenzoic acid (pABA) on  $V_2O_5$ , a potential cathode material for LIB, in a collaborative experimental (XPS) and theoretical study. The simulations using Density Functional Theory with dispersion corrections include several configurations letting different sides of the pABA interact with the  $V_2O_5$  surface. We found out that for low concentrations, the molecules prefer a lying-down configuration, while for higher concentrations they are in an up-standing configuration building a more organized SAM. From the comparison with the experimental data, a high coverage of the surface with pABA can be concluded. Hence, we infer the existence of the up-standing configuration and also the building of a well-ordered SAM.

KFM 2.2 Tue 11:30 H5

**Thermoelectric properties of novel semimetals: A case study of  $YbMnSb_2$**  — •YU PAN<sup>1</sup>, FENG-REN FAN<sup>1</sup>, XIAOCHEN HONG<sup>2</sup>, BIN HE<sup>1</sup>, CONGCONG LE<sup>1</sup>, WALTER SCHNELLE<sup>1</sup>, YANGKUN HE<sup>1</sup>, KAZUKI IMASATO<sup>3</sup>, HORST BORRMANN<sup>1</sup>, CHRISTIAN HESS<sup>2</sup>, BERND BÜCHNER<sup>2</sup>, YAN SUN<sup>1</sup>, CHENGUANG FU<sup>1</sup>, JEFFREY SNYDER<sup>3</sup>, and CLAUDIA FELSER<sup>1</sup> — <sup>1</sup>Department of Solid State Chemistry, Max Planck Institute for Chemical Physics of Solids, Dresden 01187, Germany — <sup>2</sup>Leibniz-Institute for Solid State and Materials Research (IFW-Dresden), Helmholtzstraße 20, Dresden 01069, Germany — <sup>3</sup>Materials Science & Engineering (MSE), Northwestern University, Evanston, IL 60208, USA

The emerging class of topological materials provides a platform to engineer exotic electronic structures for a variety of applications. As complex band structures and Fermi surfaces can directly benefit thermoelectric performance it is important to identify the role of featured topological bands in thermoelectrics particularly when there are coexisting classic regular bands. In this work, the contribution of Dirac bands to thermoelectric performance and their ability to concurrently achieve large thermopower and low resistivity in novel semimetals is investigated. By examining the  $YbMnSb_2$  nodal line semimetal as an example, the Dirac bands appear to provide a low resistivity along the direction in which they are highly dispersive. Moreover, because of the regular-band-provided density of states, a large Seebeck coefficient is achieved. The present work highlights the potential of such novel semimetals for high thermo-electric performance.