

## MM 39: Topical Session Theory meets Experiment IV - Batteries, Thermoelectrics and Thermal Barrier Coatings

Time: Wednesday 16:15–17:45

Location: TC 006

### Topical Talk MM 39.1 Wed 16:15 TC 006

**Electrode interfaces in organic electronics** — •KARSTEN ALBE, PETER AGOSTON, ANDRE WACHAU, MAREIKE HOHMANN, and ANDREAS KLEIN — TU Darmstadt, Inst. für Materialwissenschaft, Petersenstr. 32, D-64287 Darmstadt

Sn-doped In<sub>2</sub>O<sub>3</sub> (ITO) is a transparent conducting oxide with a high transparency in the visible range of the optical spectrum and high electrical conductivity, which is widely used as transparent electrode material for organic light emitting diodes and organic photovoltaics. Due to the orientation dependent ionization potential, a polycrystalline ITO film will exhibit a laterally varying work function, which results in an inhomogeneous charge injection into organic semiconductors when used as electrode material. Thus, a detailed understanding of the surface structure and thermodynamics is a prerequisite for optimizing the transparent electrode. In this contribution the thermodynamic stability of several experimentally observed low-index surfaces of bcc indium oxide (In<sub>2</sub>O<sub>3</sub>) are investigated by means of density functional theory calculations. The influence of hydrogen, water, n-type dopants (Sn), as well as the in-plane lattice strain are studied and compared to results of STM-studies on single crystalline samples. The computed data are also contrasted with results from photoelectron spectroscopy on magnetron-sputtered layers and explain, why the orientation dependence of the work function will become even more pronounced when oxygen plasma treatments are performed.

### MM 39.2 Wed 16:45 TC 006

**Current theoretical investigations of Li<sub>x</sub>Si as electrode materials in Li-Ion-Batteries** — •THOMAS GRUBER and JENS KORTUS — TU Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09596 Freiberg, Germany

Li<sub>x</sub>Si may be a promising anode material for lithium ion batteries. We will discuss the crystal structures of the known stable phases and will identify similar structural elements. In particular using the electron localization function (ELF) we will investigate the bonding in these structures. The main goal of our investigation is to support an understanding of the charging and discharging processes, which are directly related to the Li<sup>+</sup> transport.

For any application of Li<sub>x</sub>Si as anode material a proper understanding of the thermodynamical behavior of the material is required. The calculation of the complete phonon dispersion as function of pressures allows for the construction of the Gibbs free energy, which then gives access to specific heat or other thermodynamical data. The Gibbs free energy and derived thermodynamical quantities can be used for thermodynamical modeling of Li-ion batteries or as input for phase field simulations.

### MM 39.3 Wed 17:00 TC 006

**First Principles Study of Thermoelectric Boron-Carbide Compounds** — •KARSTEN RASIM, CHRISTIAN CARBOGNO, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin

A significant fraction of the world energy consumption goes into “waste heat”. For recovering some of it one needs to develop significantly more efficient thermoelectric (TE) materials than what is known to date. Boron-carbide based compounds have recently been proposed as promising candidates for high temperature applications, in particular due to the fact that their TE properties can be remarkably altered by adding a large variety of rare earth or transition metals [1]. In this work, we employ *density functional theory* (DFT) to assess the electronic and atomistic structure of such modified boron-carbide compounds. Thereby, we are able to identify the elemental mechanisms that determine the properties of these materials, e.g., the sign

of the majority charge carrier [1]. We further discuss how the systematic underestimation of the band gap with approximate *exchange-correlation* (XC) functionals [2] affects our results by comparing experimental data and calculations performed at various levels of theory, i.e., with LDA, GGA, and hybrid XC functionals. In particular, we comment on the implications of these findings with respect to the computational assessment of TE properties [3].

[1] T. Mori and T. Nishimura, *J. Sol. State Chem.* **179**, 2908 (2006).

[2] P. Rinke *et al.*, *New J. Phys.* **7**, 126 (2005).

[3] P. Boulet *et al.*, *Comp. Mat. Sci.* **50**, 847 (2011).

### MM 39.4 Wed 17:15 TC 006

**Computational study of structures of yttria-stabilised zirconia/strotrium titanate multilayers** — •WEI LI CHEAH and MIKE FINNIS — Imperial College London, UK

Growing interest in the field of functional oxide multilayered nano-heterostructures may be attributed to their unusual interfacial properties that are not yet fully understood. For instance, the nature of the unexpectedly high conductivity reported in a trilayer of 1-nm thick epitaxial yttria-stabilised zirconia (YSZ) film sandwiched between strontium titanate (STO) layers [1] still remains controversial. In an effort to investigate the source of conductivity in this system, we first establish an unexpected YSZ lattice within such heterosystem using a combination of techniques - a genetic algorithm in which the interatomic forces are described by classical pair potentials, and a pseudopotential-based DFT method as implemented in the plane-wave code CASTEP. We find this structure to be more stable than an anatase zirconia epitaxial lattice on STO which has been previously found as the most stable structure if yttrium dopants were not incorporated within the zirconia layer. Analysis of charge density of this new structure reveals not localised vacancies, but several small pockets of low charge densities for each expected vacancy. We examine the mobility of oxide ions in the heterosystem using classical molecular dynamics simulation and attempt to relate the results to experimental conductivity values.

[1] J. Garcia-Barriocanal *et al.*, *Science*, vol. 321, no. 5889, pp. 676-680, 2008.

### MM 39.5 Wed 17:30 TC 006

**Phase Stability in Yttria-stabilized Zirconia from First Principles** — •CHRISTIAN CARBOGNO<sup>1,2</sup>, CARLOS G. LEVI<sup>1</sup>, MATTHIAS SCHEFFLER<sup>1,2</sup>, and CHRIS G. VAN DE WALLE<sup>1</sup> — <sup>1</sup>Materials Department, University of California, Santa Barbara, CA 93106-5050, USA — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany

Zirconia based ceramics are of pivotal importance for a variety of industrial technologies, e.g., for *thermal barrier coatings* in gas and airplane turbines [1]. Naturally, the stability of such coatings at elevated temperatures plays a critical role in these applications. It is well known that an aliovalent doping of tetragonal ZrO<sub>2</sub> with Yttria, which induces oxygen vacancies due to charge conservation, increases its thermodynamic stability [1,2]. However, the atomistic mechanisms that determine the phase stability of such *Yttria-stabilized Zirconia* (YSZ) coatings are not yet fully understood [2]. In this work, we use *density functional theory* calculations to assess the electronic structure of the different YSZ polymorphs at various levels of doping. With the help of population analysis schemes, we are able to unravel the intrinsic mechanisms that govern the interaction in YSZ and that can so explain the relative stabilities of the various polymorphs. We critically compare our results to experimental measurements and discuss the implications of our findings with respect to other oxides.

[1] A. G. Evans, D. R. Clarke, and C.G. Levi, *J. Eur. Ceram. Soc.* **28**, 1405 (2008).

[2] J. A. Krogstad *et al.*, *J. Am. Ceram. Soc.* **94**, S168 (2011).