MM 54: Computational Materials Modelling VIII - Functional materials

Time: Thursday 12:00–13:00 Location: IFW D

MM 54.1 Thu 12:00 IFW D

Modeling lithium-titanium-oxide materials with structural disorder — •Saskia Stegmaier, Hendrik Heenen, Jörg Meyer, Christoph Scheurer, and Karsten Reuter — Technische Universität München, Germany

Lithium-titanium-oxides are studied intensively owing to their applications as electrode materials in rechargeable lithium-ion batteries.[1] Studies that aim for a better atomic scale understanding of the parameters which influence materials properties and dynamic processes face the challenge that materials like $Li_4Ti_5O_{12}$ (LTO) show structural disorder even in their pure-phase bulk crystal structures. A way to deal with occupational disorder in theoretical studies is the use of supercell structure models. While larger supercells allow for a better representation of the statistical distribution of atom types, they also incur computational costs that quickly become untractable for first principles methods. In consequence, density-functional theory (DFT) calculations on structural features and Li ion diffusion are in practice often carried out for rather small supercell structures. We scrutinize the reliability of such calculations and use force field and DFT methods to evaluate the configuration space for LTO materials with structural disorder.

[1] M. V. Reddy, G. V. Subba Rao, B. V. R. Chowdari, *Chem. Rev.* **2013**, *113*, 5364.

MM 54.2 Thu 12:15 IFW D

Conducting monolayers of Sodium at stacking faults in Silicon — •Benedikt Ziebarth[1,2], Matous Mrovec[1,2], Christian Elsässer[1,2], and Peter Gumbsch[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]Karlsruhe Institute of Technology, IAM-ZBS, Karlsruhe, Germany

Sodium decorated stacking faults (SFs) in Silicon were identified recently as an origin for potential-induced-degradation failure of solar-cell modules based on crystalline silicon [1]. The SFs were observed to be covered by about one monolayer of Na atoms, and this decoration was interpreted to cause local electrical short-circuits of the p-n-junction in the solar cell. In the present study such a SF in Si decorated with Na was investigated by means of density functional theory in order to elucidate its structural, diffusion and electronic properties. The Na atoms lead to a substantial elongation of Si-Si bonds across the SF. Minimum-energy-path calculations for Na atoms diffusing along the SF yield a strong dependence of the activation barrier on the degree of layer coverage of the SF with Na. In a SF with a half monolayer of Na the barrier is higher than for interstitial Na in bulk Si, whereas in a SF with a full monolayer of Na the barrier is lower by an order of magnitude. Electronic-structure calculations reveal that the Na at the SF cause defect levels in the band gap of Si which are partially filled and hence lead to electrical conduction along the SF.

[1] V. Naumann et al., phys. stat. sol. (RRL) 6, 331-333 (2012).

MM 54.3 Thu 12:30 IFW D

An ab-initio study of muscovite mica — •Anoop kishore Vatti, Mira Todorova, and Jörg Neugebauer — Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf, Germany

Muscovite mica is the most significant phyllosillicate mineral in the mica series. It is widely used as a substrate in various experiments investigating the structure of water, because it is easily cleaved yielding an atomically smooth surface structure. We perform density-functional theory calculations to study the bulk and surface properties of muscovite mica using both the Local Density Approximation (LDA) and the Generalized Gradient Approximation (PBE-GGA). Inclusion of the semi-empirical dispersion correction of Grimme (vdW-D2) turns out to be essential in order to achieve an accurate description of the system. The structural parameters,elastic constants and electronic structure of muscovite mica will be discussed, as well as the thermodynamic stability of different surface terminations.

MM 54.4 Thu 12:45 IFW D

Modeling the screening in atomically thin layers — •Ralf Hambach[1], Philipp Wachsmuth[1], Gerd Benner[2], and Ute Kaiser[1] — [1]Electron Microscopy Group of Materials Science, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Carl Zeiss Microscopy GmbH, Carl-Zeiss-Str. 22, 74447 Oberkochen, Germany

In this joint experimental and theoretical work, we investigate the electronic screening in free-standing, tilted graphene as prototype 2D material. To this end, the momentum-dependent electron energy-loss function has been measured by angular-resolved electron energy-loss spectroscopy up to 40eV using a transmission electron microscope (SALVE-I [1]). Corresponding ab-initio calculations in the framework of time-dependent density-functional theory have been performed using a plane-wave pseudopotential code [2,3]. We find very good agreement between experimental and theoretical results both for in-plane and for out-of-plane momentum transfers.

Starting from our ab-intio calculations, we assess the importance of out-of-plane excitations in the electronic screening and discuss the validity of a two-dimensional description of graphene which is often applied in model calculations by neglecting the extension in perpendicular direction. Finally, we discuss simple dielectric models to describe the anisotropy of graphene and the observed plasmon dispersion.

[1] Kaiser et al, Ultramicroscopy **111** 1246 (2011)
[2] AbInit: Gonze et al, Comp. Mat. Sci. **25** (2002)
[3] Olevano, Reining, Sottile, http://www.dp-code.org (1998)