

MM 54: Computational Materials Modelling - Defects & Interfaces II

Time: Thursday 11:45–13:00

Location: H24

MM 54.1 Thu 11:45 H24

Neural Network Studies of the Interface between Copper and Zinc Oxide — ●BJÖRN HILLER, NONGNUCH ARTRITH, and JÖRG BEHLER — Lehrstuhl für Theoretische Chemie Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany

Despite its importance as a catalyst in e.g. the methanol synthesis, the atomistic structure of copper clusters supported at zinc oxide is not fully understood. It was experimentally shown that copper entrenches into the zinc oxide upon heating. This indicates strong interactions between the copper particles and the underlying support, whose origins and implications are not resolved up to now. Theoretical studies of such systems is demanding due to the inherent problem of the lattice mismatch between the subsystems. Using standard DFT calculations one is currently limited to a few hundred atoms which only allows to investigate rather small interfaces. In the present work we explore the applicability of more efficient Neural Network potentials to describe the structural and energetic properties of a variety of copper-zinc oxide interface models.

MM 54.2 Thu 12:00 H24

Ab initio stacking fault energy calculations in Mg-Y alloys — ●ZONGRUI PEI^{1,2}, STEFANIE SANDLOEBES¹, STEFAN ZAEFFERER¹, ALEXEY DICK¹, MARTIN FRIAK¹, LI-FANG ZHU¹, SANGBONG YI³, DIETMAR LETZIG³, DIERK RAABE¹, and JOERG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen, Aachen, Germany — ³Helmholtz-Zentrum Geesthacht, Magnesium Innovation Center, Geesthacht, Germany

Pure magnesium and most commercial wrought magnesium alloys exhibit a low room temperature ductility which can be significantly increased by the addition of Y or rare earth elements (Acta Mater. 59 (2011) 429). Understanding the mechanisms causing this ductility enhancement on an atomistic and electronic-structure level would provide a systematic approach to identify alternative favorable solutes. Therefore, in order to obtain a deeper insight into the mechanisms active in the Mg-Y alloys, a quantum-mechanical (so called ab initio) study of the compositional dependence of intrinsic stacking fault (ISF) energies has been performed. Employing density functional theory (DFT) calculations, the ISF energies have been determined within the Axial Next-Nearest-Neighbour Ising (ANNNI) model. An in-depth analysis of the theoretical data shows reduced ISF energies as a direct consequence of the dramatically reduced thermodynamic stability of hexagonal Mg-Y solid solutions when the Y concentration approaches its solubility limit in Mg (Acta Mater. 60 (2012) 3011).

MM 54.3 Thu 12:15 H24

Ab initio and atomistic study of generalized stacking fault energies in Mg and Mg-Y alloys — ●LI-FANG ZHU¹, ZONGRUI PEI^{1,2}, STEFANIE SANDLOEBES¹, JOHANN PEZOLD¹, MARTIN FRIAK^{1,2}, STEFAN ZAEFFERER¹, HOWARD SHENG³, CHRIS RACE¹, BOB SVENDSEN^{1,2,4}, DIERK RAABE¹, and JOERG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen, Aachen, Germany — ³George Mason University, Fairfax, USA — ⁴Faculty of Georesources and Materials Engineering, RWTH Aachen, Aachen, Germany

Mg-Y alloys show significantly improved room temperature ductility when compared with pure Mg. We study this interesting phenomenon theoretically at the atomic scale employing quantum-mechanical and

atomistic modeling methods. Specifically, we have calculated generalized stacking fault energies for five slip systems in both elemental magnesium (Mg) and Mg-Y alloys using (i) density functional theory (DFT) and (ii) a newly developed embedded-atom method (EAM) Mg-Y potential. These calculations predict that the addition of Y results in a reduction in the unstable stacking fault energy of basal slip systems. In case of I₂ stacking fault, the predicted reduction of the stacking fault energy due to Y atoms was verified by experimental TEM measurements. We find a similar reduction for the stable stacking fault energy of the 11-22<11-23> non-basal slip system. On the other hand, other energies along this particular γ -surface profile increase with the addition of Y.

MM 54.4 Thu 12:30 H24

Surface chemistry in a full-potential QM/MM approach: making hybrids affordable — ●DANIEL BERGER¹, VOLKER BLUM², and KARSTEN REUTER¹ — ¹TU München — ²Fritz-Haber Institut der MPG

Nanostructured oxide surfaces are promising candidates for a wide range of energy and catalysis applications. When addressing corresponding functionalities through quantitative first-principles calculations, exploitation of the localized character of the chemical processes yields numerically most efficient approaches. To this end we augment the FHI-aims [1] package with a QM/MM [2] functionality, in which the nanostructure and immediate oxide surrounding is described quantum mechanically, the long-range electrostatic interactions with the support are accounted for through a polarizable monopole field, and a shell of norm-conserving pseudopotentials correctly connects the two regions. We illustrate the accuracy and efficiency of the implementation with examples from the photo-catalytic water splitting context and specifically discuss the use of charged system states to address charge transfer processes.

[1] V. Blum *et al.*, Comp. Phys. Commun. **180**, 2175 (2009)[2] N. Bernstein *et al.*, Rep. Prog. Phys., **72**, 026501 (2009)

MM 54.5 Thu 12:45 H24

Reliable Modeling of Complex Organic/Metal Interfaces — ●WEI LIU, SERGEY FILIMONOV, VICTOR G. RUIZ, MATTHIAS SCHEFFLER, and ALEXANDRE TKATCHENKO — Fritz-Haber-Institut der MPG, Berlin, Germany

The understanding of electronic properties of complex organic/metal interfaces requires a reliable method for the prediction of their structure and stability. The bonding at complex interfaces arises from delicate balance between covalent bonds, van der Waals (vdW) forces, charge transfer, and Pauli repulsion. Recently, we developed a method based on density-functional theory with vdW interactions (PBE+vdW^{surf} [1]) to accurately model adsorbates on surfaces, by a synergetic linkage of the PBE+vdW method [2] for intermolecular interactions with the Lifshitz-Zaremba-Kohn theory [3] for the dielectric screening within the substrate surface. This method is demonstrated to reliably model a multitude of small and large molecules on metal surfaces [1,4,5], leading to an accuracy of 0.1 Å in adsorption heights and 0.1 eV in binding energies with respect to state-of-the-art experiments. To demonstrate the predictive power of the PBE+vdW^{surf} method, we design a novel type of single-molecule push button switch, by carefully controlling the stability and activation barrier between a chemically bound state and a physically bound state for benzene derivatives adsorbed on metal surfaces.

[1] Ruiz, *et al.*, PRL (2012). [2] Tkatchenko and Scheffler, PRL (2009). [3] Zaremba and Kohn, PRB (1976). [4] Al-Saidi, *et al.*, Nano. Lett. (2012). [5] Wagner, *et al.*, PRL (2012).