SYMS 3: Modern developments in multiphysics materials simulations III

Time: Friday 10:15–13:00 Location: A 053

SYMS 3.1 Fri 10:15 A 053

A Neural Network Representation of High-Dimensional Potential-Energy Surfaces for Solids — •Jörg Behler[1], Davide Donadio[2], Roman Martonak[3], and Michele Parrinello[4] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Germany — [2]Department of Chemistry, UC Davis, USA — [3]Department of Experimental Physics, Comenius University, Bratislava, Slovakia — [4]Department of Chemistry and Applied Biosciences, ETH Zurich, USI-Campus Lugano, Switzerland

We present a generalized neural network scheme for the representation of high-dimensional density-functional theory (DFT) potential-energy surfaces of bulk materials. The neural network is several orders of magnitude faster to evaluate than the underlying DFT energies, while the accuracy of the potential-energy surface is essentially maintained. The method enables long-term molecular dynamics and metadynamics simulations of large systems and is applicable to crystalline and amorphous structures, as well as to the melt. The method is illustrated by studies on the pressure-induced phase transitions in silicon. The obtained results are in excellent agreement with experiment and density-functional theory.

SYMS 3.2 Fri 10:30 A 053

Cluster-Expansion formalism for arbitrary lattices — •Daniel Lerch[1], Ole Wieckhorst[1], Gus Hart[2], and Stefan Müller[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — [2]Department of Physics and Astronomy, BYU, N283 ESC, Provo, UT 84602

In the past decades the cluster-expansion (*CE*) has evolved to an important tool for the modelling of multi-scale problems for both bulk and surface systems. However, up to now CE studies have been limited to primitive lattices (e.g. *fcc, bcc, sc*). We present a CE formalism implemented in our program package UNCLE, which can expand systems with up to three components based on arbitrary non-primitive lattices (e.g. *hcp*). In the two-dimensional case this formalism allows furthermore the treatment of surface systems such as multi-site adsorption (e.g. *H on Ir(100)-5x1-H*) or alloy surfaces. The included groundstate search has been designed to minimize not only computing time but also user-interference in order to achieve correct predictions independent of chemical intuition. This makes these predictions from ab-initio studies more reliable.

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SYMS 3.3 Fri 10:45 A 053

Conformational hierarchies of weakly bonded systems: Accuracy of dispersion corrected DFT — •Alexandre Tkatchenko, Volker Blum, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

It is well known that long-range dispersion interactions, important for stabilization of, e.g., molecular crystals, biomolecules and physisorption, are badly described by state-of-the-art *xc* functionals in DFT, but naturally included in post-HF or empirically in force field simulations. We have implemented a semi-empirical C_6/R^6 correction [1,2] in the numeric atom-centered orbital based code FHI-aims [3] and obtained correction parameters by fitting to a database of high quality *ab initio* calculations [2], improving on previous results due to the more accurate basis set (0.5 kcal/mol average error for binding energies using PBE+C_6). We assess the accuracy and impact of the correction for a completely different class of systems; rather than testing the average properties of a database, we focus on conformational energy *hierarchies* of (i) $(H_2O)_n$ clusters (n=2-6), (ii) Ala$_2$ and Ala$_4$, and (iii) infinite polyalanine conformers, comparing to published post-HF results for (i) and (ii). Even though the relative energies are not changed for small H_2O clusters and Ala$_2$ compared to DFT-GGA, the impact of dispersion on the conformation hierarchy of larger systems is surprisingly large, reaching $\sim$1-4 kcal/mol for different polyalanine conformers. [1] S. Grimme, J. Comput. Chem. 25, 1463 (2004) [2] P. Jurecka et al., J. Comput. Chem. 28, 555 (2007) [3] V. Blum et al., FHI ab initio molecular simulations (FHI-aims) project.

SYMS 3.4 Fri 11:00 A 053

Magnetic Bond-order Potential: Application to Defect Behavior — •Matous Mrovec[1,2], Duc Nguyen-Manh[3], Christian Elsaesser[1,2], Peter Gumbsch[1,2], and David Pettifor[4] — [1]IZBS, University of Karlsruhe, Kaiserstr. 12, 76131 Karlsruhe — [2]Fraunhofer-Institute for Mechanics of Materials IWM,Wöhlerstr. 11, 79108 Freiburg, Germany — [3]EURATOM/UKAEA Fusion Association, Culham Science Centre, Abingdon, OX14 3DB, United Kingdom — [4]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Development of reliable interatomic potentials for simulations of structural defects in iron and iron-based materials presents a significant challenge. Energetics and structural stability of magnetic materials is strongly influenced by magnetic effects and details of the Fermi surface. These materials are therefore described rather poorly by the embedded-atom-method or Finnis-Sinclair-type potentials, which are only density dependent. We present a bond-order potential (BOP) for iron, which is based on a tight-binding bond representation. The model is able to capture the directional character of bonds present in transition metals and includes a description of magnetic effects within the Stoner model of tinerant magnetism. The constructed BOP is applied in studies of point defects, dislocations, and grain boundaries in ferromagnetic iron.

SYMS 3.5 Fri 11:15 A 053

Valence-dependent Bond-Order Potentials for Modeling Ni-based Superalloys — •Thomas Hammerschmidt, Ralf Drautz, and David Pettifor — Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, UK

The creep properties of Ni-based superalloys degrade with time due to precipitation of topologically close-packed (tcp) phases. We have compiled a structure map of the occurrence of tcp phases for binary transition-metal (TM) compounds from experimental databases. The structure map highlights the well-known role of the average d-band filling for the stability of tcp phases. Atomistic modelling of tcp stability requires extending the second-moment approximation to the electronic density of states (DOS) by including up to at least the sixth moment. We have developed an analytic bond-order potential (BOP) that systematically takes into account higher moment contributions to the DOS and depends explicitly on the valence of the TM elements. By including up to sixth-moment terms the analytic BOP is able to reproduce the structural trend across the non-magnetic 4d and 5d TM series. For the parameterization of the new BOP, we performed extensive density functional theory (DFT) calculations of the elemental and binary compound phases of Ni, the technologically important alloying element Cr, and the refractory metals Mo, Re, and W. In particular, we investigated the tcp phases A15, C14, C15, C36, μ, σ, and χ for the Ni-Cr, Re-W, Mo-Re, and Mo-W binary systems. We will discuss the structural trends of the DFT calculations and compare to the predictions of the analytic BOP within the canonical d-band model.

SYMS 3.6 Fri 11:30 A 053

Numerical Implementation of a 3D-Continuum Theory of Dislocations — •Stefan Sandfeld[1,3], Thomas Hochrainer[1,2], Peter Gumbsch[1,2], and Michael Zaiser[3] — [1]University Karlsruhe, IZBS, Karlsruhe, Germany — [2]Fraunhofer IWM, Freiburg, Germany — [3]University Edinburgh, U.K.

The growing demand for physically motivated continuum theories of plasticity led to an increased effort on continuum descriptions based on dislocations. For simplified systems of straight edge dislocations in a single slip configuration a 2-dim. theory is available (Groma 2003).

However, all attempts to transfer this method to 3-dim. systems of curved dislocations failed due to the lack of a dislocation density measure being able to reflect all dislocations as line like objects. The reason is that the Kroner tensor, as a measure for geometrically necessary dislocations (GND), comprises only a fraction of all dislocations, while the scalar density of statistically stored dislocations (SSD) contains no directional information.

This deficiency can be remedied by a recently introduced continuum theory of dislocations (Hochrainer 2006), which utilizes a generalized definition of the dislocation density tensor. Within this theory the differentiation between GND and SSD becomes dispensable. We explore this theory by a numerical implementation for the 2-dim. case of a single glide system. The effect of dislocation pile-ups at impenetrable boundaries is studied and compared to alternative approaches (e.g. Sedlacek 2003). We will show, that our method can treat arbitrary distributions of dislocation loops insinde the plastic slip channel.

SYMS 3.7 Fri 11:45 A 053

An ab-initio study of the hydrogen-bond network in crystalline α-chitin — •Michal Petrov, Martin Friák, Liverios Lymperakis, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

Light, resistant and poly-functional α-chitin is the second most abundant biological polymer. Learning/understanding how nature achieves these properties is crucial to design novel bio-inspired materials. The hydrogen-bond network formed during the crystal packing plays a key role to understand the physical properties of the material such as solubility or elasticity. A deeper understanding of chitin's unique properties has been long hindered by the lack of detailed ground-state structure information. We have therefore studied the atomic structure of crystalline α-chitin with a special focus on conformational possibilities in the hydrogen bond network. In order to properly address the full complexity of the α-chitin structure a hierarchical multischeme approach has been employed: The configurational space is first searched using force field based molecular dynamics and tight binding calculations. The most promising atomic configurations thus identified are then refined within accurate ab-initio methods. The properties of the hydrogen bond network within the rotational conformational phase space of the side chains and the influence to the energetics of α-chitin are investigated. Analyzing these results the stability of the ground-state structure as well as its strong elastic anisotropy is explained in terms of an intricate interplay between covalent and the hydrogen bonds.

SYMS 3.8 Fri 12:00 A 053

Boron-chain alloys to carry hydrogen? — •Aleksey Kolmogorov, Ralf Drautz, and David Pettifor — Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

We use *ab initio* calculations to explore the hydrogen storage potential of boron-chain Li-B alloys. Analysis of the available experimental data on the boron-chain $\text{Li}_x\text{B}_{1-x}$ compound ($x \approx 0.53$) and a high-throughput search for its most stable hydrogenated derivatives have allowed us to identify two possible LiBH (5.4 wt. % H) and LiBH_2 (10.2 wt. % H) phases. We suggest a synthesis route to obtain the new hydrides and discuss the possibility of adjusting the heats of reactions for hydrogen storage applications.

SYMS 3.9 Fri 12:15 A 053

Engineering materials-design parameters of the Mg-Li alloys from ab initio calculations — •William Art Counts, Martin Friák, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institute für Eisenforschung GmbH, Max-Planck Str. 1, D-40237, Düsseldorf, Germany

Ab initio calculations are becoming increasingly useful to engineers interested in designing new alloys because these calculations are able to accurately predict basic material properties only knowing the atomic composition of the material. In this paper, fundamental physical properties (like formation energy and elastic constants) of 11 bcc Mg-Li compounds are calculated using density-functional theory (DFT) and compared with available experimental data. These DFT-determined properties are in turn used to calculate engineering parameters like (i) specific Young's modulus (E/ρ) or (ii) bulk over shear modulus ratio (B/G) differentiating between brittle and ductile behavior. These engineering parameters are then used to identify alloys that have optimal mechanical properties needed for a light weight structural material. It was found that the stiffest bcc magnesium-lithium alloys contain about 70 at.% Mg while the most ductile alloys have 0-20 at.% Mg. The specific modulus for alloys with 70 at.% Mg is equal to that of Al-Mg alloys and slightly lower than that of Al-Li alloys.

SYMS 3.10 Fri 12:30 A 053

A Lattice-Boltzmann Model to simulate the growth of three dimensional microstructures under the influence of fluid flow — •Marcus Jainta, Michael Selzer, and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences

The effect of fluid flow on crystal growth structures is a phenomenon with particular relevance in three dimensions where solute is transported in the spatial domain and around the growing crystals. From experiments, it is well known that fluid flow dramatically alters the solidification structure during a casting process. The presence of flow admits the possibility of instabilities due to the flow itself, in addition to the well known morphological instabilities found in crystal growth. Hence, flow has an important influence on the process conditions and on the resulting material properties during the solidification from a melt. A Lattice-Boltzmann model for fluid flow is formulated and coupled with a phase-field model for multicomponent and multiphase material systems. The influence of convection on the growth process is modelled by introducing an advective term in the concentration diffusion equations. The model can be applied to multiple liquid phases with different viscosities. We discuss the numerical method and apply the parallel solver to investigate the effect of a flow field on the evolution of dendritic and eutectic solidification microstructures in two and three dimensions.

SYMS 3.11 Fri 12:45 A 053

Ab initio analysis of the carbon solubility limits in various iron phases — •Olga Kim, Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

The solubility limits of carbon in various iron phases are of critical importance for many steel-industry applications. The actual values are difficult to measure accurately in ferrite and they have so far not be determined theoretically from first principles in austenite. The solubility limits of carbon in α-, β-, γ- and δ-iron have been thus determined employing density functional theory calculations over the entire temperature range. The results show excellent agreement with experiment. The two-orders-of-magnitude higher solubility of carbon in austenite than in ferrite has been quantitatively analyzed and a complex interplay between two distinct phenomena has been found. First, the number of first nearest neighbors is higher in the fcc structure than in the bcc structure and the carbon atom is consequently more strongly bound, and secondly, the strain energy between the C-interstitial and the surrounding iron matrix is lower in the fcc lattice. The details of the actual magnetic state have not been found as important as the above mentioned two mechanisms.