MM 4: Computational Materials Modelling I - High throughput/Material discovery

Time: Monday 10:15–11:30 Location: IFW D

MM 4.1 Mon 10:15 IFW D

An automated first-principles search for solid-state lithium electrolytes — •Riccardo Sabatini and Nicola Marzari — Theory and Simulation of Materials, EPFL (CH)

In recent years much attention has been given to high-throughput techniques for materials' discovery and characterization, a complex challenge where state-of-the-art theoretical advancements meet data analytics and automated job management. We present here one of the first high-throughput projects done with our AiiDA framework (Automated Interactive Infrastructure and Database for Atomistic simulations), an open-source infrastructure built for largely automatic materials' design and discovery. Starting from the ICSD database, we build an automatic workflow to compute lithium-ion diffusion with Car-Parrinello molecular dynamics. The database subset of target lithium-containing materials is also ranked by citations number; in descending order, each structure is first optimized with a ground-state variable-cell relaxation, followed by a microcanonical simulation. Several techniques to ensure the quality of the workflow have also been developed and are discussed.

MM 4.2 Mon 10:30 IFW D

High-throughput studies multi-component Ni-rich alloys — •Michaela Höfler, Sascha B. Maisel, and Stefan Müller — Institute of Advanced Ceramics, TUHH, 21073 Hamburg, Deutschland

We present high-throughput studies of various Ni-rich alloys (Ni-Al, Ni-Ta, Ni-W, Ni-Ta-W, Al-Ni-W, Al-Ni-Ta, Al-Ni-Ta-W and Al-Ni-Ta-W) based on DFT theory guided by the cluster-expansion method. We present CE Hamiltonians, which accurately describe the ground-state behavior of the binary alloys and and discuss ternary ground-state compounds $Al_7Ni_{24}W_1$, $Al_3Ni_{12}W_1$ and $Al_3Ni_{12}Ta_1$ found to be stable in multi-component alloys across a data base of over 600 fully-relaxed DFT superstructures with up to four components. The resulting ground-states structures have substitutional $L1_2$-type order and release nearly 0.5 meV/atom of enthalpy upon formation. Our findings indicate that ternary γ'-derivates of $Al_xN_3Ta_{1-x}$ and $Al_xN_3W_{1-x}$ stoichiometries are energetically favourable over true quarternary Al-Ni-Ta-W compounds at low temperatures.

MM 4.3 Mon 10:45 IFW D

Solubility of Interstitials in Transition Metals: Knowledge Discovery using High-Throughput *ab-initio* Databases — •Ugur Aydin, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

The solubility of hydrogen in metals is decisive for a variety of phenomena incl. hydrogen embrittlement, superabundant vacancy formation and hydrogen storage. In order to design materials with tailored specific solution properties of hydrogen, a detailed knowledge about the interaction of hydrogen with the host metal is desired. We have, therefore, generated a solution enthalpy database by using an in-house developed workbench. Systematically exploring the database the elastic and chemical mechanisms governing solution enthalpies for the complete set of transition metals are derived. Several crystal structures for the host metal (bcc, fcc and hcp) and interstitial atoms have been compared. The systematic analysis resulted in a universal dependence of ΔH as a function of the lattice constant of the host metal. The trends obtained in this study provide important insights into mechanisms determining the solution enthalpy of interstitials in complex compounds.

MM 4.4 Mon 11:00 IFW D

Atomistic and inverse-analytical modeling of elastic properties of coherent nano-phases — Lei Chen[1], Li-Fang Zhu[1], •Martin Friák[1,2], Duancheng Ma[1], Christoph P. Race[1,3], Venkata S.P.K. Bhogireddy[1], Robert Spatschek[1], Bob Svendsen[1,4,5], Dierk Raabe[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Institute of Physics of Materials AS CR, v.v.i., Brno, Czech Republic — [3]Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Aachen, Germany — [4]Materials Science Centre, University of Manchester, Manchester, United Kingdom — [5]Material Mechanics, Faculty of Georesources and Materials Engineering, RWTH Aachen University, Aachen, Germany

Coherent phases precipitating in metallic matrices are known to provide e.g. a significantly increased strength and other superior mechanical properties. Nano-sized inhomogeneities of phases, that exist only when stabilized by the surrounding matrix, represent a very specific sub-class of these composites. The stabilization via internal interfaces is crucial as these phases would be thermodynamically and/or mechanically unstable as self-standing bulk. In our study we suggest the effective merging of these coherent inhomogeneities with their interfaces into a medium that is characterized by anisotropic elastic constants fulfilling conditions of mechanical stability. We combine an inverse analytical method with atomistic simulations in order to predict elastic constants and apply our approach to bcc Cu in ferritic Fe matrix.

MM 4.5 Mon 11:15 IFW D

Three-dimensional structure maps for sp-d-bonded systems — •Arthur Bialon, Thomas Hammerschmidt, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, Germany

Structure maps are an approach to identify the governing factors that determine if a mixture of elements will form a compound and which crystal structure is to be expected. Here, we present new structure maps for the sp-d-bonded systems that are footed on databases of experimentally observed crystal structures. For identifying suitable axes of the structure map we take into account both the overlap of different crystal-structure regions and the clustering of entries representing the same crystal structure. As a result, we find three most significant order parameters, in particular an electron-count, a volume and electronegativity parameter. This enables us to set up a three-dimensional structure map for the most frequently occurring crystal structures in sp-d-bonded systems that correctly predicts the ground state structure in 9 out of 10 cases.