

## MM 43: Computational Materials Modelling - Alloys II

Time: Wednesday 17:15–18:30

Location: BAR 205

MM 43.1 Wed 17:15 BAR 205

**Role of disorder in the electronic structure of thermoelectric clathrates** — ●MARIA TROPPEZ, SANTIAGO RIGAMONTI, and CLAUDIA DRAXL — Humboldt-Universität zu Berlin, Berlin, Germany

Intermetallic clathrate compounds have a huge compositional and configurational space that allows for tailoring their properties towards a high thermoelectric efficiency. For instance in  $\text{Ba}_8\text{Al}_x\text{Si}_{46-x}$ , the configuration of the Al atoms in the crystal framework drastically affects the electronic behavior [1]. This is most strikingly the case at the technologically relevant composition  $x = 16$ , whose ordered ground state is semiconducting, while disordered structures at higher energies are metallic. An in-depth understanding of this sensitivity of the electronic structure is crucial, since semiconducting behavior is a prerequisite for thermoelectric applications. In this work, we investigate the effects of disorder on the temperature-dependent electronic and structural properties. To this end, we develop a multi-scale approach, based on statistical thermodynamics combined with the cluster-expansion method [2] and *ab-initio* calculations. We discover a semiconductor-to-metal transition that is accompanied by an order-disorder phase transition at 582 K.

[1] M. Troppenz, S. Rigamonti, and C. Draxl, *Chem. Mater.* **29**, 2414 (2017).

[2] S. Rigamonti, *et al.*, CELL: python package for cluster expansions with a focus on complex alloys. URL: <https://sol.physik.hu-berlin.de/cell>

MM 43.2 Wed 17:30 BAR 205

**High-temperature thermodynamics of Ni alloys with machine learning** — ●NATALIYA LOPANITSYNA and MICHELE CERIOTTI — École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Many thermodynamic properties of metals show a pronounced temperature dependence that is challenging to obtain fully from *ab initio*. However, to achieve agreement between theoretical considerations and experiment, temperature-dependent contributions also should be taken into account. One of the problems is the absence of an accurate and efficient technique to obtain the correction. It becomes even more evident for properties such as the excess free energy associated with a solid-liquid interface which requires a number of atoms and simulation times unaccessible with electronic structure calculations. Interatomic potentials could be used to overcome computational expenses encountered in relation to *ab initio* methods. In this paper, to achieve high accuracy in the description of the interatomic interaction, we trained a neural network to approximate the potential energy surface defined by a solution of the Kohn Sham equation of DFT and incorporated it into free energy sampling techniques to quantify anharmonic effects appearing at high temperatures. We present a wide range of properties computed at finite temperature including elastic properties, bulk modulus, melting temperature, formation energies of single point defects, surface tension for nickel chosen as a representative of metal used for high-temperature applications. Additionally, we show the importance of having an accurate underlying interatomic potential by comparing fitted NNp to potentials reported in the literature.

MM 43.3 Wed 17:45 BAR 205

**Machine trained interatomic potentials for multicomponent alloys** — ●KONSTANTIN GUBAEV<sup>1</sup>, YUJI IKEDA<sup>2</sup>, FRITZ KÖRMANN<sup>1,2</sup>, EVGENY PODRYABINKIN<sup>3</sup>, and ALEXANDER SHAPEEV<sup>3</sup> — <sup>1</sup>Materials Science and Engineering, Delft University of Technology, 2628 CD, Delft, The Netherlands — <sup>2</sup>Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — <sup>3</sup>Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Nobel St. 3, Moscow, 143026, Russia

Accurate density-functional theory (DFT) calculations have become an indispensable tool in computational exploration and design of multicomponent alloys as high entropy alloys (HEAs). The vastly unknown compositional and structural phase space of HEAs as well

as the methodological obstacles related to the description of finite-temperature properties challenges the computational limits of standard DFT approaches and reveals the need for more efficient techniques.

Here we present DFT trained machine-learning potentials (MLIPs) as efficient force-fields for investigating finite-temperature properties of multicomponent alloys. The MLIP construction for a given alloy is performed within an iterative framework comprising the phase space sampling and subsequent MLIP training in an automated manner. As a result, MLIPs reconstructing the DFT atomic forces and total energies with unprecedented speed/accuracy combination are obtained. We demonstrate the approach by performing finite-temperature molecular-dynamics simulations to assess elastic properties of a set of bcc TiZrHfTa<sub>x</sub> HEAs.

MM 43.4 Wed 18:00 BAR 205

**Multi-scale Cluster Dynamics Modelling of Guinier–Preston Zone Formation in binary Al–Cu Alloys** — ●TOBIAS STEGMÜLLER and FERDINAND HAIDER — Universität Augsburg, Institut für Physik, Universitätsstr. 1, 86159 Augsburg

The understanding of precipitation kinetics in modern age hardening aluminium alloys is, due to its significance on materials properties, of great technical interest. The link between ageing temperature and the evolution of the size distribution of precipitates is the key influence on material parameters like strength, hardness or corrosion resistance. Therefore the modelling of precipitation processes comes into focus to enable a quantitative prediction of the impact of ageing processes. For this purpose we developed a multi-scale model for the precipitation in binary alloys and tested it on the formation of Guinier–Preston zones (GPZ) in Al–Cu.

The approach results in the construction of a meso-scale Cluster Dynamics (CD) model, which is able to predict the evolution of the size distributions of the GPZ for different ageing temperatures and alloy compositions. Atomistic lattice Monte Carlo (MC) simulations were used to derive the necessary kinetic and thermodynamic input for CD. Finally, the smallest scale level includes density functional theory to derive a Cluster Expansion for the binary Al–Cu system, which provides the interaction parameters for our MC simulations. In addition, to validate the CD model, kinetic MC simulations on the formation of GPZ were conducted. The construction of the model as well as simulation results will be presented.

MM 43.5 Wed 18:15 BAR 205

**Implementation of the coordination corrected enthalpies method into AFLOW** — ●RICO FRIEDRICH<sup>1</sup>, MARCO ESTERS<sup>1</sup>, COREY OSES<sup>1</sup>, DEMET USANMAZ<sup>1</sup>, CORMAC TOHER<sup>1</sup>, and STEFANO CURTAROLO<sup>1,2</sup> — <sup>1</sup>Center for Autonomous Materials Design, Duke University, USA — <sup>2</sup>Materials Science, Electrical Engineering, Physics and Chemistry, Duke University, USA

The AFLOW database and software leverages *ab initio* calculations for autonomous materials design [1]. The predictive power critically relies on accurate formation enthalpies – quantifying the thermodynamic stability of a compound. For polar materials such as chalcogenides (*e.g.* oxides), pnictides (*e.g.* nitrides), and halides, standard semi-local DFT leads to errors of several hundred meV/atom [2,3].

We have recently developed the "coordination corrected enthalpies" (CCE) method yielding highly accurate room temperature formation enthalpies with mean absolute errors down to 27 meV/atom [3]. The approach is also capable of correcting the relative stability of polymorphs – an advantage versus earlier schemes. Here, we introduce a tool where users can input a structure file of their system and receive the CCE corrections, or even the CCE formation enthalpies if pre-calculated LDA, PBE or SCAN formation energies are provided. The results can be used for the computational design of polar compounds such as battery materials, defect systems, and high-entropy phases.

[1] S. Curtarolo *et al.*, *Comput. Mater. Sci.* **58**, 218 (2012).

[2] V. Stevanović *et al.*, *Phys. Rev. B* **85**, 115104 (2012).

[3] R. Friedrich *et al.*, *npj Comput. Mater.* **5**, 59 (2019).