MM 65: Topical session: Data driven materials design - uncertainity approaches

Time: Thursday 15:45–16:30 Location: BAR 205

MM 65.1 Thu 15:45 BAR 205

Validation and uncertainty assessment of bond-order potentials for transition metals — •Matous Mrovec, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Univerität Bochum

Bond-order potentials (BOPs) present a bridge between electronic and atomistic modeling. They are based on the tight-binding (TB) approximation, but the exact diagonalization of the Hamiltonian is replaced by an approximate evaluation of the local densities of states, which leads to a real-space formalism and linear-scaling computation of the energy and forces for a system of interacting atoms. The BOP formalism can be carried out using either a numerical integration or an analytical expansion of the response functions.

In this work we present a detailed comparison of the k-space TB with the numerical and analytic BOPs for several transition metals, and assess the differences of the three approaches. The tests are carried out not only for properties of bulk phases but particular focus is given to crystal defects which are often used to validate the accuracy and reliability of interatomic potentials for transition metals.

MM 65.2 Thu 16:00 BAR 205

Numerical Quality Control for DFT–based Materials Databases — C. Carbogno[1], K. S. Thygesen[2], •B. Bieniek[1], C. Draxl[4], L. Ghiringhelli[1], A. Gulans[4], O. T. Hofmann[3], K. W. Jacobsen[2], S. Lubeck[4], J. J. Mortensen[2], M. Strange[2], E. Wruss[3], and M. Scheffler[1] — [1]FHI Berlin, Germany — [2]DTU, Lyngby, Denmark — [3]TU Graz, Austria — [4]HU Berlin, Germany

Electronic-structure theory has become an invaluable tool in materials science. Still, the precision of different approaches has only recently been scrutinized thoroughly (for the PBE functional) using extremely accurate numerical settings [1]. Little is known, however, about code- and method-specific deviances and error bars that arise under numerical settings commonly used in actual calculations. We shed light on this issue by systematically investigating the deviances in total and relative energies as function of typical settings for basis sets, **k**-grids, etc. for 71 elemental [1] and 81 binary solids in four different electronic–structure codes. On the basis of the observed trends, we propose analytical models for the estimation of error bars. They are also cross-validated using data obtained from the NoMaD Repository [2]. Eventually, we discuss the extensibility of our approach towards more complex materials properties, e.g., band gaps, and its general applicability in the context of computational materials databases.

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[1] K. Lejaeghere *et al.*, Science **351** (2016).
[2] *https://nomad-repository.eu*

MM 65.3 Thu 16:15 BAR 205

Sensitivity analyses for large sets of density functional theory calculations — •Jan Janssen, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Over the last years methodological and computational progress in atomistic simulations has substantially improved the predictive power in materials design. However to compare the simulation results with experimental data, it is necessary to quantify the various sources of uncertainty. We therefore leverage the capabilities of our recently developed Python based workbench PyIron, to implement stochastic sensitivity analyses with the aim to differentiate model errors, statistical errors and systematical errors.

For each error we estimate the convergence gradient based on our sensitivity analyses combine it with the individual cost function of the convergence parameters and derive an algorithm for automated convergence. This approach allows us to quantify the precision not only of the energy of an individual ab initio calculation but moreover for derived quantities of sets of ab initio calculations.