MM 44: Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century

Big Data II

Time: Thursday 10:15–11:45   Location: H 0107

MM 44.1 *(64)*   Thu 10:15   H 0107
Towards a Roadmap of Chemical Space — •JOHANNES MARGRAF and KARSTEN REUTER — Technische Universität München

Data-driven research in materials science and chemistry is typically focused on the properties of individual compounds. If the value of some property is known for a representative part of chemical space, the remaining values can be estimated by interpolation. In this context, it is essential to understand what compounds make up the chemical space of interest. This can be trivial to define (e.g. all binary octet semiconductors) or require significant effort (e.g. all organic molecules up to a certain size). With this contribution, we want to shift the focus from individual compounds to chemical reactions. This means that chemical space is transformed from a list of compounds to a network of reactions connecting them (i.e. a map).

To this end, we will show how the space of chemical reactions can be constructed and organized in a systematic and exhaustive manner. We will further discuss how these reaction networks can be applied in the prediction of reaction mechanisms. Finally, we will compare how machine learning of reaction energies performs in reaction and compound space.

MM 44.2 *(369)*   Thu 10:30   H 0107
CritCat (H2020): Rational design of catalyst materials from first-principles — •JAAKKO AKOLA — Tampere University of Technology, Finland — NTNU Trondheim, Norway

The H2020-project CritCat aims to provide solutions for the substitution of critical metals, especially rare platinum groupmetals (PGMs), used in heterogeneous and electrochemical catalysis. CritCat explores the properties of ultra-small transition metal (TM) nanoparticles to achieve optimal catalytic performance with earth-abundant materials. The emphasis is on industrially-relevant chemical reactions and emerging energy conversion technologies in which PGMs play an instrumental role, particularly in the context of hydrogen energy. The goal is to tailor optimal nanoparticle catalysts for selected (electro)chemical reactions.

The CritCat project includes all the aspects for rational catalyst design including novel catalyst synthesis, characterization, and performance testing together with large-scale computational simulations of the relevant catalysts, substrates and model reactions using the latest computational methods. The DFT data is collected in a descriptor database and used for materials screening at later stages. We have developed new machine learning algorithms for neural network (NN) force fields for generating catalyst structures, descriptor-based efficient hydrogen adsorption site scanning and prediction, and effective charge and energy level prediction based on xyz-files. The new tools pave way for much more efficient catalyst simulations with DFT accuracy.

MM 44.3 *(393)*   Thu 10:45   H 0107
Machine Learning Structural Descriptors on Nanocluster Catalysts — •MARC JÄGER[1], EIAKI MOROOKA[1], and ADAM FOSTER[1,2] — [1]Aalto University, Helsinki, Finland — [2]Kanazawa University, Japan

Scientists have advanced significantly in producing nanoparticles with defined composition, size and morphology in the last decade. Due to this and because of their remarkable properties, nanoclusters have gained attention in heterogeneous catalysis. Nanoclusters differ from bulk metal behaviour, their catalytic properties are sensitive to changes in size and morphology. Nanoparticles like molybdenum disulfide are known to catalyze the hydrogen evolution reaction (HER). The combinatorial and structural space of nanoclusters is vast, so extensive modelling is difficult. Structural descriptors are used to describe the geometry of an adsorption site and to predict properties which indicate a high catalytic activity, in particular the hydrogen adsorption free energy. We analysed the performance of state-of-the-art structural descriptors (SOAP, MBTR and ACSF). Simulations can provide energetic and kinetic analysis of HER using DFT. The vast amount of possible nanoclusters, all potential candidates for catalysing the HER, requires reduction and interpolation of DFT calculations. This is tack-

led by merging the combinatorial space with the chemical compound space and applying machine learning on diverse datasets.

MM 44.4 *(351)*   Thu 11:00   H 0107
Automatic Selection of Atomic Fingerprints for Machine-Learning Potentials — •GIULIO IMBALZANO — École polytechnique fédérale de Lausanne, Lausanne, Switzerland

Machine learning of atomic-scale properties is revolutionizing the way simulations are performed, making it possible to evaluate interatomic potentials with first-principles accuracy, at a fraction of the cost. The accuracy, speed and reliability of a machine-learning potential, however, depend strongly on the way atomic configurations are represented before being used as inputs. The raw Cartesian coordinates are typically transformed in "fingerprints" that are designed to better encode the symmetries of the problem and the physics of the interactions. I discuss an automatic protocol to select a reduced number of fingerprints out of a large set of candidates, based on the intrinsic correlations of the training data. This procedure can greatly simplify the construction of neural-network potentials that strike the best balance between accuracy and computational efficiency, and has the potential to accelerate by orders of magnitude the evaluation of Gaussian Approximation Potentials based on the Smooth Overlap of Atomic Positions kernel.

MM 44.5 *(146)*   Thu 11:15   H 0107
Data-driven assessment of the transferability of effective interatomic potentials — •Y.V. LYSOGORSKIY, T. HAMMERSCHMIDT, and R. DRAUTZ — Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Many materials properties are directly accessible with high-precision by quantum-mechanical calculations using density-functional theory (DFT). However, the computational costs of the DFT calculations make many important materials properties difficult to calculate. To tackle this problem interatomic interaction potentials are widely used. A large number of interatomic potentials is available for a wide range of chemical elements and their mixtures. A central difficulty for applying potentials is the typically very limited information about their reliability for a particular simulation. We performed high-throughput calculations using DFT and interatomic potentials in order to investigate the transferability of interatomic potentials statistically. The results of our calculations are collected in a specially designed database for further analysis. The consequent statistical and correlation analysis of properties and their deviations with respect to reference values allow us to quantify the errors and transferability of interatomic potentials.

MM 44.6 *(113)*   Thu 11:30   H 0107
Data-driven approach to accelerate the development of Bond-Order-Potentials — •JAN JENKE, APARNA P.A. SUBRAMANYAM, ALVIN LADINES, THOMAS HAMMERSCHMIDT, and RALF DRAUTZ — ICAMS Ruhr-Universität Bochum, Bochum, Germany

Interatomic potentials provide a means to simulate extended length and time scales that are outside the reach of ab-initio calculations. However, the transferability of interatomic potentials to atomic environments which were not included in the parameterization of the potential is often unknown and a (re-)parameterization usually very time consuming. We suggest a data-driven approach to overcome these problems for the development of tight-binding (TB) based bond-order-potentials (BOP). The parameterization is mapped to a multi-dimensional optimization problem, which is initialized by a comprehensive database of TB parameters across the periodic table. Using a 2d structure map we systematically sample the possible atomic environments during the parameterization process. This also allows us to predict and analyse the transferability to structures which were not included in the parameterization process. We demonstrate that our method accelerates the development of BOPs with a transparent parameterization process and at the same time provides a direct and quantitative measurement of transferability.