MM 18: Topical session: Integrated computational materials engineering for design of new materials IV

Time: Tuesday 10:15–11:45 Location: H39

Topical Talk MM 18.1 Tue 10:15 H39

Robust crystal-structure prediction with structure maps — •Thomas Hammerschmidt — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

The prediction of the crystal structure of a material from only its chemical composition is one of the key challenges in materials design. The most common strategies are (i) the search for the energetically most favourable crystal structure by explicit atomistic calculations and (ii) the identification of descriptors that allow extrapolations from known materials to unknown compounds. A promising approach of the second kind are structure maps that chart the bonding chemistry of known compounds. I will discuss two structure maps and motivate their descriptors that are based on physically intuitive functions of the number of valence electrons, the atomic volume and the electro-negativity. The first example, a structure map for complex intermetallic phases, is set up by electronic-structure considerations. This two-dimensional map correctly predicts the crystal structure of precipitates in multi-component Ni-base and Co-base superalloys. The second example is a three-dimensional structure map derived by a systematic cluster analysis of experimentally observed compounds of sp-block elements and transition metals. This map reaches a predictive power that is close to standard density-functional theory calculations. The identified descriptors remain valid for off-stoichiometric compounds and separate binary and ternary crystal-structure prototypes.

MM 18.2 Tue 10:45 H39

Better (random) walking through chemistry: how not to get lost in vast configurational spaces — •Chiara Panosetti[1], Konstantin Krautgasser[1], Dennis Palagin[2], Karsten Reuter[1], and Reinhard Maurer[3] — [1]Technische Universität München — [2]University of Oxford — [3]Yale University

Ab initio structure prediction can systematically aid the computational discovery and rational design of new materials, as well as providing interpretative insights when atomistic details are difficult to resolve experimentally. However, global geometry optimization –the method of choice for finding chemically relevant (meta-)stable structures– is rarely applied to large-scale systems. The main challenge lies in the necessity of efficient ways to traverse configurational spaces in which the number of minima explodes with system size. We recently proposed an approach to global screening in chemically meaningful subspaces [1]. Following the *fil rouge* of the exploitation of chemically motivated trial moves, we now extend it to the study of organic molecules on surfaces –by suitably imposing partial constraints– and to complex interfaces with variable or unknown stoichiometry –by applying strategies to alleviate the strain of newly generated structures upon grand-canonical particle insertion. A selection of prototypical results will be presented (a retinoic acid analogue on Au(111) and metal-silicon clusters growth) to illustrate how all relevant portions of chemical space can be accessed with this approach, whereas “conventional” sampling often even struggles to produce sensible structures besides the starting geometry at all.

[1] Nano Lett., doi: 10.1021/acs.nanolett.5b03388 (2015)

MM 18.3 Tue 11:00 H39

Chemically-motivated coordinates and their potential role in efficient materials structure search — •Konstantin Krautgasser[1], Chiara Panosetti[1], Dennis Palagin[2], Karsten Reuter[1], and Reinhard Maurer[3] — [1]Technische Universität München — [2]University of Oxford — [3]Yale University

Finding energetically favorable, chemically relevant structures is a main challenge for computational materials discovery. Especially for reactions in heterogeneous catalysis and the design of hybrid inorganic-organic interfaces we generally encounter a structural complexity that cannot be treated by a manual search of minimum energy structures. We propose automatically created delocalized internal coordinates (DICs) that adapt to the local chemistry as a key tool to enable more efficient global structure screening. DICs can be straightforwardly constructed for gas-phase or adsorbed systems, molecular aggregates, crystals and complex interfaces. The ability to enforce arbitrary constraints facilitates the search in chemically-motivated subspaces. We present the construction procedure and shape of DIC displacements for a representative gas-phase system, an organic adsorbate, and a dense molecular overlayer. We implemented this in a Python package (`winak`) that can be interfaced with a multitude of electronic structure and molecular mechanics modelling tools. The modular framework of the package enables direct community contribution and connection of these coordinates with a number of different global optimization procedures.

MM 18.4 Tue 11:15 H39

Tight-binding parameterizations across the periodic table — •Jan Jenke[1], Alvin Ladines[1], Thomas Hammerschmidt[1], David G. Pettifor[2], and Ralf Drautz[1] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]Materials Modelling Laboratory, Department of Materials, University of Oxford, UK

Tight-binding (TB) parameters may be obtained from density functional theory (DFT) by projecting the DFT wave functions on the TB minimal basis. We create a comprehensive database of TB parameters for all dimers of sp- and sd-valent atoms using the Harris-Foulkes wave function as reference. We demonstrate that the Hamiltonian matrix elements of the intrinsically non-orthogonal and the Loewdin-transformed orthogonal TB model, as well as the overlap matrix elements, can be satisfactorily fitted using a single functional form. This enables us to compute the bond energy, promotion energy and repulsive energy within the TB bond model and to carry out a systematic analysis of hybridization and screening effects. We extract trends of the TB parameters across the periodic table and verify the quality of the parameterizations for bulk structures.

15 min. coffee break