MM 40: Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century

Big Data I

Big Data in Materials Science: Managing and exploiting the raw material of the 21st century organized by Claudia Draxl (Humboldt University, Berlin, Germany) and Peter Fratzl (MPI of Colloids and Interfaces, Golm, Germany)

Time: Wednesday 15:15–16:45 Location: TC 006

Topical Talk MM 40.1 Wed 15:15 TC 006

Novel high-entropy carbides discovered by synthesizability descriptors — •Stefano Curtarolo — Duke University, Durham NC, USA — Fritz Haber Institut, Berlin, Germany

High-entropy materials have attracted considerable interest due to their combination of potentially unique properties and promising technological applications. Predicting their formation from previously known parameters remains the major hindrance to the discovery of new systems. In this seminar, we introduce a descriptor - entropy forming ability - for predicting the synthesizability of such systems from first principles calculations. The formalism, based on the energy distribution spectrum of randomized calculations, captures the accessibility of equally-sampled states near the ground state and quantifies configurational disorder potentially leading to high-entropy homogeneous single-phases. The methodology is used to seek for disordered refractory 5-metal carbides | potential systems for ultra-high temperature applications. The descriptor correctly predicts a set of candidates that are experimentally synthesized as novel high-entropy homogeneous phases, validating the ansatz of the model. The method has the potential to accelerate the search and development of high-entropy crystalline systems by rationally combining first principles approaches with experimental synthesis.

MM 40.2 Wed 15:45 TC 006

First-Principles Thermodynamics of ZrO_2 at a Hybrid Level Using a Machine-Learned Potential — •Emre Ahmetcik, Angelo Ziletti, Matthias Scheffler, Christian Carbogno, and Luca M. Ghiringhelli — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany

Due to their outstanding electronic and thermal properties, zirconia-based materials are used in a wide range of industrial applications, e.g., as catalyst support, as ionic conductor, and as thermal barrier coating [1]. Computational studies of its thermodynamic properties have hitherto relied on LDA/GGA-type functionals. However, it is well known that the exchange-correlation functional significantly affects the outcome of the calculations for this material [2]. We overcome this limitation by building a machine-learned Gaussian Approximation Potential [3] from a small number of first-principles calculations performed with a hybrid exchange-correlation functional. This allows us to simulate the dynamics of zirconia in supercells containing several hundreds of atoms and for several nanoseconds. By this means, we are able to obtain the phase diagram of ZrO_2 and to understand the mechanism that drive the monoclinic-tetragonal phase-transition.

[1] A. Evans, D. Clarke, and C. Levi, J. Eur. Ceram. Soc. 28, 1405 (2008)
[2] C. Carbogno *et al.*, Phys. Rev. B 90, 1441 (2014)
[3] A. P. Bartok *et al.*, Phys. Rev. Lett. 104, 136403 (2010)

MM 40.3 Wed 16:00 TC 006

First-Principles High-Throughput Study of Thermal Lattice Expansion Coefficients — •Maja-Olivia Lenz, Florian Knoop, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The thermal lattice expansion of bulk solids plays an important role in practical applications. Nonetheless, little of the respective data is tabulated to date ($< 2,000$ entries on Springer Materials) and the existing few first-principles data is in part obtained within arguable approximations [1]. We have used the quasi-harmonic approximation [2] to compute the thermal expansion for more than 1,000 materials from first principles using our recently developed Python framework HIGH-aims. Besides performing the necessary structure relaxations and phonon calculations, this framework also handles automatized convergence of numerical settings and evaluates different exchange-correlation functionals for cross-checking. We discuss the practical challenges of this approach and the trends observed across structural and chemical space. Eventually, we discuss opportunities to apply machine-learning techniques to predict different thermal properties of new, possibly so far unknown materials.

[1] C. Toher *et al.*, *Phys. Rev. B* **90**, 17417 (2014).
[2] S. Biernacki and M. Scheffler, *Phys. Rev. Lett.* **63**, 290 (1989).

MM 40.4 Wed 16:15 TC 006

High Throughput Screening for Novel Non-magnetic Antiperovskites — •Harish K. Singh, Ingo Opahle, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, Otto-Berndt-Straße 3, 64287 Darmstadt, Germany

Analogous to ABO_3 perovskite compounds, antiperovskite materials are one of the most commonly explored materials in recent years, due to many intriguing physical properties, such as superconductivity, solid electrolytes in batteries, thermoelectricity etc. In this work, we focus on nonmagnetic antiperovskite in the $Pm\bar{3}m$ space group with chemical formula M_3XY, where M and X are s-block, d-block (except Cr-Ni), and p-block elements (except noble gas, Po and At), and Y is B, N and C. This results in approximately 9,500 compounds. We carried out high throughput density functional theory calculations to evaluate the stability, including thermodynamical, mechanical, and dynamical stabilities, which are obtained by evaluating the formation energy together with the convex hull, elastic constants, and phonon dispersion, respectively. The distance from the convex hull is evaluated by considering all possible decompositions into binary and ternary compounds from the Materials Project database. Many novel non-magnetic antiperovskites compounds are predicted which satisfy all the above mentioned stability criteria, with interesting electronic properties awaiting for further experimental validation.

MM 40.5 Wed 16:30 TC 006

Finding new superconductors: doped insulators and the construction of computational descriptors — •Antonio Sanna[1], Jose' A. Flores-Livas[2], Henning Glawe[4], Kay Dewhurst[1], Gianni Profeta[3], and E.K.U. Gross[1] — [1]MPI of microstructure physics, Halle — [2]University of Basel — [3]Universita' de L'Aquila — [4]MPI for the structure ad dynamics of matter, Hamburg

Searching for thermodynamically stable new superconductors is computationally quite demanding. But thermodynamic stability is not a necessary requisite for a system to exist and to be of technological and scientific relevance. Simple cases of non thermodynamically stable materials are doped insulators that, at high doping, can become metallic and even superconductors. We show a few interesting cases we have recently investigated: phosphorene and water under pressure.

This type of ab-initio approaches are however computationally expensive and can not easily be applied to the investigation of large databases of materials or within accelerated material design algorithms. In this case a viable strategy could be to try to construct *superconductivity descriptors*, meant to be computationally cheap quantities (on the order of a Kohn-Sham DFT calculation) that, still, are able give a reliable indication of the superconducting coupling in a system. We review some past ideas, present a few new descriptors and validate them towards the actual ab-initio calculation.