CPP 18: Topical Session: Data Driven Materials Science - Materials Design II (joint session MM/CPP)

Time: Monday 11:45–13:00 Location: BAR 205

CPP 18.1 Mon 11:45 BAR 205

Versatile Bayesian deep-learning framework for crystal-structure recognition in single- and polycrystalline materials — •Andreas Leitherer, Angelo Ziletti, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Physical properties of a given material are directly related to its structure. In particular, in polycrystalline materials the location and nature of grain boundaries are crucial features determining their properties. For instance, mechanical characteristics of steels are strongly influenced by grain boundaries. In this work, we propose *strided pattern matching* which is a framework using single-crystal classification to investigate polycrystals. Accessible crystal-structure identification methods are either very robust – but can treat only few classes – or include a large number of classes – but are not very robust. We use a Bayesian neural network in combination with the smooth-overlap-of-atomic-positions (SOAP) descriptor, allowing us to classify, robustly and without any predefined threshold, more than 100 prototypes including not only bulk but also two- and one-dimensional materials (e.g., fullerenes). Furthermore, we are able to quantify the uncertainty in the model predictions. As an example for polycrystal investigation, we apply our model to recognize an ordered $L1_2$ phase in a disordered fcc matrix. This serves as a model system for precipitate detection in Ni-based superalloys, which are materials used in aircraft engines.

CPP 18.2 Mon 12:00 BAR 205

Parametrically Constrained Geometry Relaxations for High-Throughput Materials Science — •Maja-Olivia Lenz[1], Thomas A. R. Purcell[1], David Hicks[2], Stefano Curtarolo[1,2], Matthias Scheffler[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Department of Materials Science and Mechanical Engineering, Duke University, Durham, USA

Exploiting crystal symmetries is a common technique to accelerate and improve electronic-structure calculations. However, this method usually fails when the global symmetry is broken, e.g., in materials with defects. We present a relaxation scheme that uses parametric geometry constraints to allow symmetry conservation at all levels [1]. We demonstrate how it can be used to relax metastable structures that are otherwise poorly addressable. Using the example of polarons in MgO [2], we showcase the ability to relax structures with local symmetry breaking with known distortion patterns. The flexibility of our constraints is particularly useful to accelerate high-throughput searches for novel materials. A performance study on several hundreds of different materials throughout the structural space has been done using the AFLOW Library of Crystallographic Prototypes [3]. The assignment of prototypes is helpful not only to enable user-friendly searches in materials databases like NOMAD Archive but also to describe and refine terms and concepts in a prospective materials ontology.

[1] M.-O. Lenz, *et al.*, accepted in Npj Comput. Mater. (2019).
[2] S. Kokott, *et al.*, New J. Phys. **20** (3):33023 (2018).
[3] M. J. Mehl, *et al.*, Comp. Mater. Sci. **136**, S1 (2017).

CPP 18.3 Mon 12:15 BAR 205

Combining ab-initio and data-guided approaches for refractory multi-principal element alloys design — •Yury Lysogorskiy[1], Alberto Ferrari[2], and Ralf Drautz[1] — [1]AMS, ICAMS, Ruhr University Bochum, Bochum, Germany — [2]Delft University of Technology, Delft, Netherlands

Refractory multiple principal element alloys (MPEA) nominally consist of several elements of the groups IV-VI at near-equal compositions in a single crystalline bcc phase that is characterized by exceptional high-temperature mechanical properties and a very high melting point. In this work we introduce a computationally tractable and accurate method, based on first-principles calculations and alloy modelling, to predict phase stability in MPEAs at arbitrary compositions. We reconstruct the complete phase diagram of the prototypical refractory MPEAs Mo-Nb-Ta-W and detect the regions where the formation of a solid solution is favorable at a given transition temperature. We then extend the modeling of temperature dependent properties with supervised machine learning (ML) and combine these results to a ML model for Vickers hardness, trained on experimental data from literature, to identify out-of-equiatomic composition regions of lower solid-solution formation temperature and higher hardness.

CPP 18.4 Mon 12:30 BAR 205

Data-Efficient Machine Learning for Crystal Structure Prediction — •Simon Wengert[1], Gábor Csányi[2], Karsten Reuter[1], and Johannes T. Margraf[1] — [1]Chair of Theoretical Chemistry, TU Munich, Germany — [2]Department of Engineering, University of Cambridge, UK

The combination of modern machine learning (ML) approaches with high-quality data from quantum mechanical (QM) calculations can yield models with an unrivalled accuracy/cost ratio. However, such methods are ultimately limited by the computational effort required to produce the reference data. In particular, reference calculations for periodic systems with many atoms can become prohibitively expensive. This trade-off is critical for crystal structure prediction. Here, a data-efficient ML approach would be highly desirable, since screening a huge space of polymorphs with small stability differences requires the assessment of a large number of trial structures with high accuracy.

In this contribution, we present tailored hybrid-ML models that allow screening a wide range of crystal candidates while adequately describing the subtle interplay between intermolecular interactions such as H-bonding and many-body dispersion effects. This is achieved by enhancing a physics-based description of long-range interactions —for which an efficient implementation is available— with a short-range ML model trained on high-quality first-principles reference data. The presented workflow is broadly applicable to different molecular systems, without the need for a single periodic calculation on the reference level of theory.

CPP 18.5 Mon 12:45 BAR 205

Uncovering Anharmonicity in Material Space — •Thomas Purcell, Florian Knoop, Chuanqi Xu, Matthias Scheffler, Luca Ghiringhelli, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Identifying materials with ultra-low thermal conductivities κ is the pivotal challenge in the development of more efficient thermoelectric devices. One strategy to achieve this goal is to find materials with a high level of anharmonicity, and therefore reduced phonon lifetime and κ. To help discover such materials, we calculate the anharmonicity of materials ranging from simple binary compounds to complex perovskites using the high-throughput framework *FHI-vibes* [1]. The framework automatically generates an accurate harmonic model for a material's vibrational properties, from which we determine its anharmonicity by statistically comparing the harmonic and *ab initio* forces of thermally displaced structures. Our screening not only demonstrates that anharmonicity is more prevalent in material space than previously thought, but also shows that the developed metric strongly correlates with various thermal properties. Using classes of simple binaries as an example, we show that the anharmonicity of a material can be related to its atomic, bulk, and harmonic properties via the sure independence screening and sparsifying operator (SISSO) approach [2], thus facilitating an even more efficient screening.

[1] https://vibes.fhi-berlin.mpg.de
[2] R. Ouyang, *et al. Phys. Rev. Mat.* **2**, 083802 (2018)