MM 60: Topical session: Data driven materials design - machine learning

Time: Thursday 12:00–13:15 Location: BAR 205

MM 60.1 Thu 12:00 BAR 205

Finding descriptors for material properties from billions of candidates via compressed sensing: accurate prediction of crystal structures and band gaps from only chemical composition — •Runhai Ouyang, Emre Ahmetcik, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Identifying the key physical parameters (termed descriptor) determining the target material properties is a critical step toward material discovery and rational design. Thus far, systematic methods for the descriptor identification are not well established. In particular, it has been suggested that good descriptors should both yield an accurate prediction and be physically interpretable [L. M. Ghiringhelli,*et al.*, PRL **114**, 105503 (2015)]. In this talk, we present a systematic scheme for descriptor identification based on sure independent screening [J. Fan and J. Lv, J. R. Statist. Soc. B **70**, 849 (2008)] and compressed sensing [E. Candès and M. B. Wakin, IEEE Signal Proc. Mag. **25**, 21 (2008)]. The scheme starts with automatic building of the "feature spaces", i.e. all offered candidate descriptors, and the feature space may contain billions of options. The employed combination of sure independent screening and compressed sensing provides an efficient scheme for identifying the best low-dimensional descriptor. The approach is demonstrated for the important problems of crystal-structure and band-gap prediction. This work received funding from The Novel Materials Discovery (NOMAD) Laboratory, a European Centre of Excellence.

MM 60.2 Thu 12:15 BAR 205

Representing energy landscapes by combining neural networks and the empirical valence bond method — •Sinja Klees[1], Ramona Ufer[2], Volodymyr Sergiievskyi[2], Eckhard Spohr[2], and Jörg Behler[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Duisburg-Essen, D-45141 Essen, Germany

In recent years, artificial neural networks (NNs) have become a powerful method to develop reactive interatomic potentials for a wide range of systems. Due to their high flexibility, they allow to interpolate reference energies and forces obtained from electronic structure calculations, without the introduction of any constraint to the functional form. However, the construction of NN potentials can become computationally very demanding due to the high dimensionality of the configuration space, which needs to be mapped. Combining NN potentials with the empirical valence bond (EVB) method offers a promising approach to derive the potential energy surface of complex systems with substantially reduced effort, since the size of the reference structures can be strongly decreased by employing the EVB method to combine smaller fragments in a physically meaningful way. Preliminary results will be discussed and compared to density functional theory data.

MM 60.3 Thu 12:30 BAR 205

Automatic crystal-structure classification using X-ray diffraction patterns and convolutional neural networks — •Angelo Ziletti, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

With the advent of high-throughput materials science, millions of calculations are now available to the scientific community (http://nomad-repository.eu and references therein). A reliable identification of the lattice symmetry in these calculations is a crucial first step for materials characterization and analytics. Current methods based on space-group symmetries require a user-specified threshold, and are unable to detect "average" symmetries for defective structures (e.g., with point defects, and/or strain). We propose a new machine-learning based approach to automatically classify periodic structures according to their Bravais lattice. First, we calculate the X-ray diffraction patterns, from which a classifying model is then learned using a convolutional neural network. This method is applied to crystal-structure classification of 3d, 4d, and 5d transition metal alloys, also containing vacancies. We show that our deep-learning model can correctly classify more than 99% of the crystal structures. Moreover, contrarily to other (common) methods, it does not require any tolerance threshold and provides a reliable probabilistic classification also for heavily defective structures. Our approach has been implemented in the NOMADsim package of the Novel Materials Discovery (NOMAD) Analytics-Toolkit (https://analytics-toolkit.nomad-coe.eu). This work received funding from the NOMAD Laboratory, a European Center of Excellence.

MM 60.4 Thu 12:45 BAR 205

Optimizing Materials Properties with Machine Learning Techniques: A Case Study on Hard-Magnetic Phases — •Johannes J. Möller, Georg Krugel, Wolfgang Körner, Daniel F. Urban, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

Machine Learning (ML) is an emerging field in materials science, in which a numerical model is built in order to predict a certain feature, for instance a materials property. The model building is typically based on a (large) data set of e.g. crystal structures or chemical compositions, for which the property is already known. The beauty of this approach is that it not only allows us to predict the properties for unknown compositions, but also to determine the composition that optimizes the desired property. Furthermore, ML models are inherently independent of how the original input data sets were determined, i.e. by experiments or by simulations.

In this presentation, we use ML techniques to predict optimal chemical compositions for new hard-magnetic materials. The underlying data set was determined in a combinatorial high-throughput-screening approach based on density-functional theory calculations [Drebov et al., New J. Phys. 15 (2013); Körner et al., Sci. Rep. 6 (2016)]. The developed ML models allow us to predict promising structure-composition combinations for substitutes of state-of-the-art materials like $Nd_2Fe_{14}B$ with similar intrinsic ferromagnetic properties but no or less amounts of critical rare-earth elements. Finally, we discuss possible perspectives for further applications of ML in materials science.

MM 60.5 Thu 13:00 BAR 205

A theoretical tool to predict the nature of the 4f states of Ce compounds — •Heike C. Herper[1], Tofiq Ahmed[2], John M. Wills[2], Igor di Marco[1], Inka Locht[1], Anna Delin[3], Alexander V. Balasky[2], and Olle Eriksson[1] — [1]Department of Physics and Astronomy, Uppsala University, Sweden — [2]Center for Integrated Nanotechnologies, LANL, USA — [3]KTH Royal Institute of Technology, Stockholm, Sweden

Cerium is the most abundant rare earth. Ce compounds are used in many applications and therefore different materials properties are needed. Since these properties are widely determined by the electronic structure the understanding of the degree of localization of the 4f electron is essential. Aiming to classify the Ce compounds regarding to their itinerant character we studied the hybridization function Δ of more than 350 data sets taken from the ICSD. The hybridization function has been calculated from first principles using a full-potential code [1]. We show that the strength of Δ evaluated in this way allows conclusions about the level of 4f localiztion. The results are consistent with the experimental information regarding the degree of 4f localization, for the studied materials. A strong anti-correlation between the size of Δ and the volume of the systems has been observed. The information entropy is about 0.42 which means a high predictive power that could be used to tailor new materials with desired properties.

[1] J. M. Wills et al, Full-Potential Electronic Structure Method, Springer series solid state science **167** (2010).

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