MM 55: Topical session: Data driven materials design - structure maps

Time: Thursday 10:15–11:45 Location: BAR 205

MM 55.1 Thu 10:15 BAR 205

Materials discovery with artificial intelligence — •Gareth Conduit and Philipp Verpoort — Department of Physics, University of Cambridge, UK

We have developed a computational tool that employs deep learning with neural networks to discover new materials. The tool combines databases of experimental results with Density Functional Theory calculations to get high accuracy across a broad range of compositions. This enables us to propose materials that are most likely to fulfil multivariate targets. This holistic approach to materials design has allowed us to propose four new nickel-base alloys for use in jet engines, whose properties have been experimentally verified, new Lithium-ion battery cathode materials, and titanium alloys.

The neural network approach to materials modelling can also assess the integrity of materials data. We have exploited this capability to automatically validate and correct entries in a commercial metal alloy and polymer database.

MM 55.2 Thu 10:30 BAR 205

Quantification of different atomic environments by a 2d structure map — •Jan Jenke[1], Aparna Puchakayala Appaiah Subramanyam[1], Thomas Hammerschmidt[1], David G. Pettifor[2], and Ralf Drautz[1] — [1]ICAMS Ruhr-Universität Bochum, Bochum, Germany — [2]University of Oxford, Oxford, United Kingdom

The assessment of the geometric (dis)similarity of crystal structures is a central requirement to facilitate information on structural stability with applications ranging from machine-learning of DFT data to the development of effective interaction models. The moments theorem relates the moments of the local electronic density of states to the local geometric environment of an atom. The moments of the electronic density of states therefore may be viewed as descriptors from which the local atomic surrounding of an atom may be reconstructed. By restricting our analysis to the two most important moments we map the phase space of possible atomic surroundings onto a two-dimensional space. Each local atomic environment corresponds to a point on the map and the entirety of all atomic environments forms a two-dimensional structure map. We apply the structure map to determine differences in the local atomic surrounding of known crystal structures, random structures, transformation paths and molecular dynamics trajectories. We show that our two-dimensional structure map leads to a natural separation of crystal structures that one would argue are very different while crystal structures that are similar are grouped close together. We suggest that our structure map is able to sample the space of atomic surroundings in a formal locally but at the same time intuitive way.

MM 55.3 Thu 10:45 BAR 205

Uncovering structure-property relationships of materials by subgroup discovery — •Mario Boley[2], Bryan R. Goldsmith[1], Jilles Vreeken[2], Matthias Scheffler[1], and Luca M Ghiringhelli[1] — [1]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]Max Planck Institute for Informatics, Campus Mitte, 66123 Saarbrücken, Germany

Data analytics applied to materials-science data often focuses on the inference of a global prediction model for some physical or chemical property of interest for a given class of materials, such as activation barriers or binding energies. However, the underlying mechanism for some target property could differ for different materials within a large pool of materials-science data. Consequently, a global model fitted to the entire dataset may be difficult to interpret and may well hide or incorrectly describe the actuating physical mechanisms. In these situations, local models would be advantageous to global models. Subgroup discovery (SGD) is presented here as a data-mining approach to find interpretable local models of a target property in materials-science data. We first demonstrate that SGD can identify physically meaningful models that classify the crystal structures of 82 octet binary semiconductors as either rocksalt or zincblende. The SGD framework is subsequently applied to 24 400 configurations of neutral gas-phase gold clusters with 5 to 14 atoms to discern general patterns between geometrical and physicochemical properties. This work received funding from The Novel Materials Discovery (NOMAD) Laboratory, a European Center of Excellence.

MM 55.4 Thu 11:00 BAR 205

Predicting lattice parameters of ternary compounds by compressed sensing — •Benedikt Hoock[1,2], Santiago Rigamonti[1], Luca Ghiringhelli[2], Matthias Scheffler[1,2], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Data analytics is emerging as a new branch of materials science enabling the interpolation and even (moderate) extrapolation of high-level computational results. In our present work, we demonstrate the successful prediction of lattice parameters for a set of 438 group-IV zincblende ternary compounds from density-functional theory (DFT) results. We use a compressed-sensing based method that combines the least absolute shrinkage and selection operator (LASSO) and ℓ_0-regularized optimization on a feature space consisting of basic features and a large range of simple mathematical combinations of them. The basic features comprise atomic and dimer DFT data as well as properties of relaxed tetrahedral clusters. We achieve a root mean square error of ~ 0.04 Å(~ 0.4 %) for the fit and a similar prediction accuracy, as estimated by a leave-10%-out cross-validation.

MM 55.5 Thu 11:15 BAR 205

Compressed-Sensing Models for the Prediction of the (Meta-)Stability of Octet Binaries — •Emre Ahmetcik, Runhai Ouyang, Christian Carbogno, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

Predicting the ground-state and metastable crystal structures of materials from just knowing their composition is perhaps the most important challenge in materials science. In a recent showcase study [1], a compressed-sensing based methodology was introduced to identify the *descriptors* (nonlinear functions of atomic input features) that best describe and predict the relative stability of zincblende versus rocksalt octet binary compounds. In this work, we have extended this approach to describe the relative stability and energy differences between eight different polymorphs of the octet binary materials, so that an accurate prediction of their ground and metastable states becomes possible. We discuss how this is tackled by introducing a new class of descriptors that map the geometry of different structures into a well defined scalar (the "reduced" Madelung energy) and a multi-objective optimization (the simultaneous minimization of the prediction error of all formation-energy differences among the eight considered polymorphs).

This work received funding from The Novel Materials Discovery (NOMAD) Laboratory, a European Centre of Excellence.

[1] Ghiringhelli *et al.*, PRL **114**, 105503 (2015).

MM 55.6 Thu 11:30 BAR 205

Self-organisation Map (SOM) on 3D Electrostatic Potential Surface (EPS) — •Baichuan Sun, Michael Fernandez, and Amanda Barnard — Molecular & Materials Modelling, Data61 CSIRO, Door 34 Goods Shed, Village St, Docklands, VIC 3008, Australia

State-of-art of Deep Learning (DL) algorithm are having tremendous impact on Big Data analytics across all scientific fields, and Material Science (MS) is no exception. A combination of computational chemistry simulations and DL techniques requires a hybrid computation/data research workflow, which represents a revolutionary approach to MS studies. There is a gap between data of nanomaterial*s quantum chemistry information and its analytics with DL frameworks which stems from difficulties in representing quantum mechanical properties in such a data structure that could be suitable for artificial neural networks. At the Molecular & Materials Modelling Laboratory we are evaluating the efficiency of visualising nanoparticles' 3-D Electrostatic Potential Surface (EPS) with Self-organising Maps (SOM), and their modelling with DL framework. Self-organisation Map (SOM) classifies high-dimensional data into low-dimensional space without supervision, while retaining the intrinsic topological relationship of the dataset. This algorithm is ideal for representing 3D molecular electrostatic potential surface (EPS) with a single 2D snapshot. The 2D image could possibly be fed into conventional classifier models, to correlation the EPS with other corresponding chemical properties of the molecules.