# MM 29: Data Driven Materials Science: Big Data and Work Flows – Electronic Structure

Time: Wednesday 11:45–13:00 Location: SCH A 251

MM 29.1 Wed 11:45 SCH A 251

**Band Gap and Formation Energy Inference of Solids using Message Passing Neural Networks** — •Tim Bechtel, Daniel Speckhard, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Berlin, Germany

Graph-based neural networks and, specifically, message-passing neural networks have shown great promise in predicting physical properties of solids. Here, we target three tasks, formation energy regression, metal-non-metal classification, and band gap regression, using data from the AFLOW materials database [1]. In order to find optimal hyperparameters and model architecture, we perform a neural architecture search on the band gap regression task, using a random search algorithm. The model is based on a message passing neural network with edge updates [2], and provides users with uncertainty estimates via Monte-Carlo dropout. We analyze the domain of applicability of the model, for different space group symmetries, atomic species, and corrections applied to the underlying calculation. While we obtain overall excellent results, the model struggles to accurately predict oxide materials. We find that the uncertainty in different domains reflects the model's predictive performance.

[1] S. Curtarolo et al., Comput. Mater. Sci., 58 (2012), pp. 227-235.
[2] P.B. Jørgensen et al., Preprint at arXiv:1806.03146 (2018).

MM 29.2 Wed 12:00 SCH A 251

**Predicting electron density using a convolutional neural network** — •Jae-Mo Lihm[1,2,3], Wanhee Lee[4], and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul, Korea — [4]Department of Applied Physics, Stanford University, California, USA

Machine-learning methods are being widely applied to computational materials science. Most applications of machine learning in electronic structure calculations focus on learning the total energy and forces, while few works study the prediction of electronic properties. In this work, we develop a machine-learning model for predicting electron density using the convolutional neural network, a standard machine-learning method for image processing. We train the neural network using the electron density calculated from density functional theory. We show that the trained neural network can successfully predict the electron density of systems that were not included in the training set, bypassing the need for the self-consistent density functional theory calculation.

MM 29.3 Wed 12:15 SCH A 251

**Chemical ordering and magnetism in CrCoNi Medium Entropy Alloy** — •Sheuly Ghosh[1], Vadim Sotskov[2], Alexander Shapeev[2], Jörg Neugebauer[1], and Fritz Körmann[1,3] — [1]Max-Planck-Institut für Eisenforschung GmbH — [2]Skolkovo Institute of Science and Technology — [3]Delft University of Technology

The equiatomic CrCoNi medium entropy alloy is a prototypical multiple-principal element alloy (MPEA), exhibiting many superior mechanical properties. Short-range order (SRO) is known to affect the thermodynamic phase stability as well as mechanical and magnetic properties of MPEA alloys. In CrCoNi also, the presence of SRO and its impact on different aspects has been intensively discussed in various studies. In our recent study, we identified the ground-state ordered structure for this alloy combining *ab initio* calculations and on-lattice machine-learning interatomic potentials. Based on these studies, an ordered $Cr(Ni,Co)_2$ phase ($MoPt_2$-type) was found. In present work, we further discuss the stability of the newly identified ordered structure and compare them with the previously suggested ones, particularly with respect to magnetism, local atomic relaxation energies as well as volume fluctuations.

MM 29.4 Wed 12:30 SCH A 251

**Charge-dependent Atomic Cluster Expansion** — •Matteo Rinaldi, Anton Bochkarev, Yury Lysogorskiy, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Bochum, Germany

The atomic cluster expansion (ACE) [1,2,3] has proven to be a valuable tool to parametrize complex energy landscapes of pure elements and alloys outperforming popular approaches based on limited body-order descriptions. However, due to the local nature of the many body basis, it is inherently near-sighted. Therefore, long range interactions, such as electrostatics, are ignored in the description. Here, we introduce charge-dependent ACE to be able to tackle the missing electrostatic contributions. This formalism is based on the QEQ charge equilibration scheme from Rappe et al.^[4], where partial charges are obtained by equalizing atomic electronegativities and imposing charge conservation. Moreover, atomic electronegativities and hardness are considered as dependent on the local atomic environment. We demonstrate that our approach yields atomic charges in agreement with those obtained from popular partitioning schemes, such as Mulliken and Hirshfeld, including periodic and non-periodic systems, together with an accurate reproduction of the potential energy landscape. This work opens the possibility to model charge transfer and dielectric response within the increasingly popular ACE framework.

[1] R. Drautz, Phys. Rev. B 99, 014104 [2] Y. Lysogorskiy et al., npj Comput Mater 7, 97 (2021) [3] R. Drautz, Phys. Rev. B 102, 024104 [4] Rappe, J. Phys. Chem. 1991, 95, 8, 3358*3363

MM 29.5 Wed 12:45 SCH A 251

**A machine-learned interatomic potential for silica and mixed silica-silicon systems** — •Linus C. Erhard[1], Jochen Rohrer[1], Karsten Albe[1], and Volker L. Deringer[2] — [1]Institute of Materials Science, TU Darmstadt, Darmstadt, Germany — [2]Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, Oxford, United Kingdom

The interface between silica and silicon has enormous relevance in various applications, including semiconductors and novel battery materials. However, atomistic modeling of this interface is a challenge due to the different charge states of silicon and the limitations of classical interatomic potentials. To overcome these limitations, we introduce a machine-learning-based interatomic potential based on the non-linear atomic cluster expansion (ACE) for various Si-O phases. This model is based on the previously developed database for silica [1], which was substantially extended by active learning. The new model shows improved performance for high-pressure silica and is also able to describe silica surfaces. Moreover, the use of the ACE formalism enables us to reach more than 100 times longer time or larger length scales compared to the Gaussian approximation potential (GAP). Finally, the potential is able to describe off-stoichiometric mixtures of Si and $SiO_2$. This capability is used to investigate the nanostructure of silicon monoxide.

[1] Erhard et al. A machine-learned interatomic potential for silica and its relation to empirical models. npj Comput Mater 8, 90 (2022)