Session of Focus Materialchemie – Wednesday, **24.01.2024** 16:00 – @ Seminarraum Lehar 02 (TU-Wien, Getreidemarkt 9, BC, OG. 02, room A46) – join us on ZOOM (ID: 983 0066 2349)

Understanding Uncertainties in Neural-Network Force Fields

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Atomistic simulation is currently experiencing a paradigm shift. Namely, by promising a combination of DFT-like accuracy with fast computation times, machine learned force-fields (MLFF) are increasingly replacing traditionally parametrized force-fields, thus enabling precise simulation of large atomic systems. However, one major open question in the development of such potentials is how the training structures can be picked in a generic and clever way. This should lead to a potential with high accuracy in the relevant domain of structure space while keeping redundancy in the training database low. An option to achieve this would be by applying an active learning strategy accompanied with data reduction methods. [1]

In a recent published study, Unglert et al. [2] showed that the silicon phase diagram can be predicted accurately by combining the nested sampling algorithm with our in-house developed MLFF NeuralIL [3] trained on an already existing hand-crafted silicon database [4]. Building upon that study, in this work it will be illustrated that it is possible to construct the training database solely by applying an active learning strategy. On top of that, different iterations of the active-learned MLFF will be analyzed and learned lections will be discussed.

References:

[1] Exploring chemical and conformational spaces by batch mode deep active learning. Zaverkin Viktor, Holzmüller David, Steinwart Ingo and Kästner Johannes. Digital Discovery. DOI:10.1039/D2DD00034B

[2] Neural-network force field backed nested sampling: Study of the silicon p-T phase diagram. Unglert Nico, Carrete Jesús and Pártay Livia B. and Madsen Georg K. H. Phys. Rev. Mater. DOI:10.1103/PhysRevMaterials.7.123804

[3] A Differentiable Neural-Network Force Field for Ionic Liquids. Hadrián Montes-Campos, Jesús Carrete, Sebastian Bichelmaier, Luis M. Varela, and Georg K. H. Madsen. Journal of Chemical Information and Modeling. DOI: 10.1021/acs.jcim.1c01380

[4] Machine Learning a General-Purpose Interatomic Potential for Silicon. Albert P. Bartók, James Kermode, Noam Bernstein, and Gábor Csányi. Phys. Rev. X. DOI:10.1103/PhysRevX.8.041048