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Transferability of DFT surrogate models: Temperature and system size

Thursday 15 September 2022 15:15 (30 minutes)

While Density Functional Theory (DFT) is the most common tool for the investigation of materials under extreme conditions, its scaling behavior with respect to both system size and temperature makes large scale simulations challenging. Yet, progress in this regard would enable accurate modeling of planetary interiors or radiation damage in fusion reactor walls. One possible route to alleviate these scaling problems is through the use of surrogate models, i.e., machine-learning models. These are trained on DFT data and are able to reproduce DFT observables at comparable accuracy, but negligible computational cost. In order to actually be useful for such investigations, existing models need to be able to work across length scales and be transferable within desired temperature ranges. Here we show how models based on local mappings of electronic structure information [1], implemented in the Materials Learning Algorithms (MALA) package 2 can be trained on small number of atoms and select temperatures, yet perform accurately when used to make predictions for extended systems within a range of temperatures.

[1]: J. A. Ellis et al., Phys. Rev. B 104, 035120, 2021

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