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Learning many-body potential energy landscape for analysis of neutron scattering data

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For the discovery of new materials in the field of energy storage, catalysis, and biological processes, molecular dynamics (MD) simulations are an indispensable computational tool. We can achieve highly accurate representations of the potential energy landscape of diverse molecular systems with ab-initio molecular dynamics (AIMD) simulations, but at the cost of high computational time which limits typical applications to 100s of atoms and time scales of ~100ps. This is where machine learning potentials can be used to capture the underlying physics from first principles, where electrons are treated quantum mechanically, while still reaching long simulation times relatively cheaply.

We introduce a workflow for the analysis of neutron scattering data that trains several deep-learning based many-body potentials and interatomic forces from ab-initio reference calculations. Further, to gauge the accuracy of such potentials with classical MD programs, we use the inelastic neutron scattering (INS) spectra as the performance metric. An INS spectra serves as one of the most stringent tests of theory (such as density functional theory), since the model has to predict not only the correct structure but also the correct vibrational dynamics. We use a genetic algorithm to optimize several hyperparameters used in this workflow. For different molecular samples, we successfully demonstrate that our workflow can replicate the experimental INS spectra measured at SNS.

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