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Machine Learned Interatomic Potentials for Extreme Environments

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Classical molecular dynamics (MD) is in principle an ideal tool to investigate the long-time evolution of materials in extreme environments, as ab initio-based MD simulations remain limited to very short time. While modern machine learning MD potentials report errors on the order 1 meV/atom, these errors are only typical of configurations that are similar to those found in the training set used to fit the potential, and transferability to genuinely new configurations remain limited. This poses a challenge to the accuracy of long-time MD simulations for two reasons: i) transition rates are exponentially sensitive to energy barriers, and ii) saddle configurations form a very small subset of the whole configuration space and are unlikely to appear in traditional hand-crafted datasets, or even as part of conventional active-learning approaches. We propose a large-scale automated workflow to develop and validate transferable machine learned interatomic potentials (MLIP) for long-time simulations in extreme environments. The workflow is implemented in the pyiron workflow framework, developed in our group, which accelerates the rapid prototyping and up-scaling of computational materials science workflows up to the latest generation of Exascale Computers. Finally, we apply the resulting MLIPs to calculate bulk phase stabilities and the stability of defect phases.

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