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# Shallow ensembles for practical uncertainty quantification in equivariant neural network potentials

Machine-learning interatomic potentials (MLPs) efficiently approximate the potential energy surface given by an underlying first-principles method, for example density-functional theory, enabling simulations at previously unachievable time and length scales. However, for practical applications, it is critical to know when predictions can be relied upon, and when additional data is needed. We evaluate the recently proposed shallow ensembles [1] approach to uncertainty quantification for the state-of-the-art So3krates MLP [2]. As a prototypical usecase, we choose molecular dynamics simulations of CuI, where dynamic formation of interstitials prevents ahead-of-time training.

1: Kellner and Ceriotti, Mach. Learn. Sci. Technol. **5** (2024)
2: Frank, Unke, Müller, and Chmiela, arXiv:2309.15126 (2024)

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