Multi-fidelity machine learning interatomic potentials for charged point defects

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Abstract

Machine learning interatomic potentials (MLIPs) have emerged as powerful tools for materials discovery, achieving quantum-mechanical accuracy for pristine systems at reduced computational cost [1,2]. However, their application to defective systems where coordination environments and electronic structures deviate from pristine bulk materials remains challenging. This is especially severe for charged defects, where charge-dependent atomic relaxations and energy landscapes push beyond the local descriptors that most MLIPs rely on. In this talk, I first show that state-of-art foundation models [3,4,5] trained on bulk materials fail to reliably identify defect ground-states. To address this, we develop a joint model with global charge embeddings that successfully identifies ground-state configurations and accurately predicts defect charge transition levels for multiple charged defects. We further employ a multi-fidelity training strategy that combines a high volume of low-cost PBE data with selective high-quality HSE data. This reduces the computational cost of achieving hybrid-functional accuracy by three orders of magnitude, while resulting in a robust model that identifies global minima missed in low-precision searches. The resulting defect-capable force fields act as fast surrogate models that can describe the properties governed by the underlying potential energy surface. Our work lays the groundwork for future defect foundation models capable of generalising across materials, charge states, and levels of theory.

References

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