A FRAMEWORK FOR A GENERALISATION ANALYSIS OF MACHINE-LEARNED INTERATOMIC POTENTIALS

YANGSHUAI WANG*

ABSTRACT

The presence of defects in crystalline materials significantly affects their mechanical and chemical properties, hence determining defect geometry, formation energies, and mobility is a fundamental problem of materials modelling. Machine-learned interatomic potentials (MLIPs) have since been developing rapidly and beginning to have significant impact on many practical systems, which promise to bridge the significant gap in accuracy and capability between ab initio electronic structure models and classical mechanistic models. In this work, we propose a rigorous generalisation analysis of the material properties (defect geometry and formation energy), investigating the error propagation from fitting MLIPs on a small training domain to predicting on a large simulation domain. We (i) give the rigorous existence results for the equilibrium of multiple point defects; (ii) establish the *a priori* error estimates of geometry error and error in formation energy in terms of the separation distance of defects and the matching conditions between the reference models and MLIPs, and (iii) demonstrate how to use these matching conditions to construct practical MLIPs for multiple defects systems.

* Department of Mathematics, University of British Columbia.

* yswang2021@math.ubc.ca