Ab initio construction of full phase diagram

While several studies confirmed that machine-learned potentials can provide accurate free energies for determining phase stabilities, the abilities of MLPs for efficiently constructing a full phase diagram of multicomponent systems are yet to be established. In this work, by employing neural network interatomic potentials, we demonstrate construction of the MgO-CaO eutectic phase diagram including liquid phases based on free energy calculation methods. In particular, the phase diagram predicted by the NNP trained on SCAN functional closely follows the experimental data. We believe that this work paves the way to fully ab initio calculation of phase diagrams. This work was published at Physical Review Materials 2022, 6, 113802.