

Recent developments in computer power have enabled prediction of crystal structures using ground state energies based on density functional theory. This is done by means of global optimization techniques that explore low-lying energy structure in addition to the putative global minimum. The major obstacle to this approach is that the number of structures increases exponentially with respect to the number of atoms in the unit cell, therefore, a thorough exploration of energy landscape including large supercells is not computationally feasible. Replacing density functional theory by interatomic potentials can be a solution to this problem provided the interatomic interactions are described accurately. We present a sort of interatomic potentials based on machine learning that enables us to predict novel crystal structures with a computational cost that is a fraction of those accomplished by density functional methods.