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A first-principles interatomic potential via perturbative theory
XINYUAN AI, CHRIS MARIANETTI, Columbia University — Here we propose a new approach for constructing a first-principles interatomic potential based upon a Taylor series expansion in clusters of the atomic displacements. While the number of clusters is very large in general, group theory can be used to generate a tractable number of clusters in materials with sufficiently high symmetry. A large dataset of perturbed structures which randomly samples the irreducible cluster phase space is constructed and computed in density functional theory. The cross validation score is then used to determine which clusters should be retained in the expansion. This method is then benchmarked on a one-dimensional atomic chain. Excellent agreement is achieved within a large range of atomic displacements in addition to large lattice strains. Additionally, one can recover the phonons as a function of strain. Further application of the method to two and three dimensional materials are also presented.

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