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.