

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

A slave cluster expansion for obtaining ab-initio interatomic potentials XINYUAN AI, Department of Physics, Columbia University, CHRIS MARIANETTI, Department of Applied Physics and Applied Mathematics, Columbia University — Here we propose a new approach for performing a Taylor series expansion of the first-principles computed energy of a crystal as a function of the nuclear displacements. We enlarge the dimensionality of the existing displacement space and form new variables (i.e. slave clusters) which transform like irreducible representations of the point group and satisfy homogeneity of free space. Standard group theoretical techniques can then be applied to deduce the non-zero expansion coefficients *a priori* at a given order, and the translation group can be used to contract the products and eliminate terms which are not linearly independent. While the expansion coefficients could likely be computed in a variety of ways, we demonstrate that finite difference is effective up to fourth order. We demonstrate the power of the method in the strongly anharmonic system PbTe. All anharmonic terms within an octahedron are computed up to fourth order. A proper linear transform demonstrates that the vast majority of the anharmonicity can be attributed to just two terms, indicating that a minimal model of phonon interactions is achievable. The ability to straightforwardly generate polynomial potentials will allow precise simulations at length and time scales which were previously unrealizable.

Xinyuan Ai
Department of Physics, Columbia University

Date submitted: 15 Nov 2013

Electronic form version 1.4