Phonon Optimized Potentials

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Molecular dynamics (MD) simulations have been extensively used to study phonons and gain insight, but direct comparisons to experimental data are often difficult, due to a lack of empirical interatomic potentials (EIPs) for different systems. As a result, this issue has become a major barrier to realizing the promise associated with advanced atomistic level modeling techniques. Here, we present a general method for specifically optimizing EIPs from ab initio inputs for the study of phonon transport properties, thereby resulting in phonon optimized potentials (POPs). The method uses a genetic algorithm (GA) to directly fit to the key properties that determine whether or not the atomic level dynamics and most notably the phonon transport are described properly.

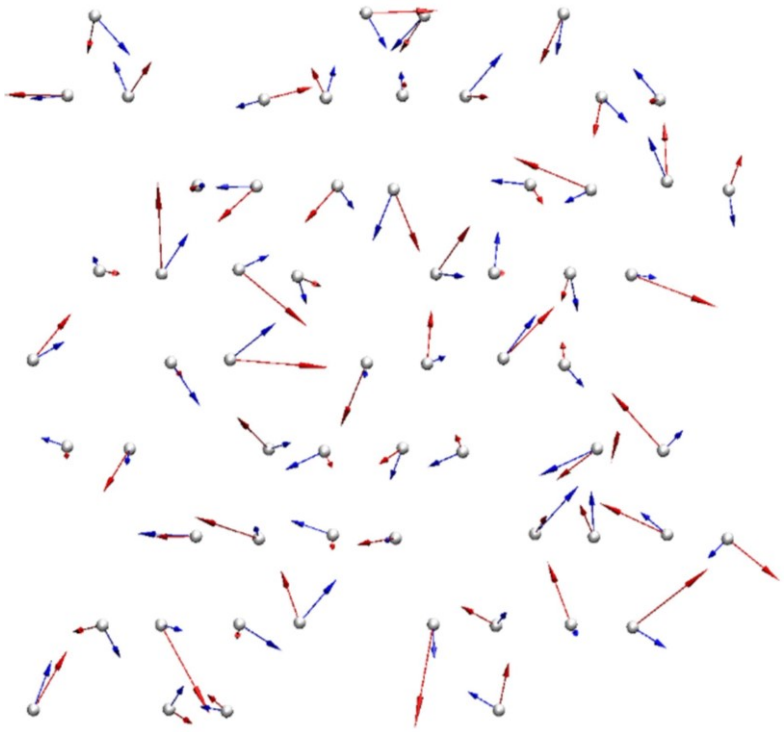

Fig. 1: A silicon crystal with atoms randomly displaced from equilibrium, along with ab initio forces (blue vectors) compared to forces from a commonly used empirical potential (red vectors). This error is drastically reduced using the POPs code and method discussed herein, resulting in interatomic potentials that can accurately reproduce phonon properties.