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Phonon Optimized Potentials ANDREW ROHSKOPF, ASEGUN HENRY, Georgia Institute of Technology, ATOMISTIC SIMULATION AND ENERGY RESEARCH GROUP TEAM — Atomistic simulations can be used to predict thermal properties with atomic insight, mainly via molecular dynamics (MD) simulations where the atomic forces are calculated every time step to predict atomic motions. Accurate dynamics requires an accurate method of sampling the potential energy surface (PES). For practical atomistic studies of thermal properties across relevant length ($>10^3$ nanometers) and time scales ($>10^2$ nanoseconds), a model of the PES with the following Requirements is needed: (1) PES sampling must be fast (<0.01 second/atom). (2) PES sampling must be chemically accurate (<1 kcal/mol). (3) Requirement 2 must be transferrable to thermally relevant regions of the PES. Quantum mechanical (QM) methods such as density functional theory (DFT) satisfy Requirements 2 and 3, but fail Requirement 1. Many attempts to bypass the computational costs of QM include empirical interatomic potentials (EIPs). Many EIPs fail Requirement 2 and 3, however. We have therefore created a machine learning program that can parameterize any EIP to satisfy Requirements 2 and 3. These phonon optimized potentials reproduce phonon dispersion relations, and therefore thermal properties, quite well.

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