Multibody expansions: An ab initio based transferable potential for computational thermodynamics[1]

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Ab initio based techniques provide by far the most comprehensive and accurate details for computational thermodynamic and structure evolution studies. The computational complexity of these methods precludes the application of such first-principal analysis to configurations beyond a few hundred atoms. But in many cases, long-ranged and many-body interactions are necessary to model the energy accurately. We utilize a multibody based representation of the potential energy landscape to accurately represent these interactions in a computationally efficient manner. The many-body expansion is constructed via accurate sparse grid interpolation over a large database of ab-initio cluster energies. This framework results in the construction of transferable potentials that can be seamlessly integrated into various MD and MC platforms. We will illustrate the accuracy, efficiency and transferability of the proposed potential expansion using several computational thermodynamics based applications including the computation of stable structures of binary alloys.

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