On the development of weighted many-body expansions using ab-initio calculations for predicting stable crystal structures[1]

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Calculation of stable structures of alloys, clusters, surfaces and molecules from first-principles is an important step towards design of materials with exceptional properties. The effect of structural relaxations in alloys is described using multi-body energy expansion formalism. N-body potentials in the multi-body expansion are computed from energies of isolated clusters, which in turn, are calculated from empirical potentials or self-consistent quantum mechanical calculations. Convergence characteristics of multi-body expansions (MBE) are improved by weighting energies obtained from various truncations of many-body expansion in a new method called weighted MBE (wMBE). It is shown that multi-body expansions of many-atom systems can be efficiently constructed using interpolation of isolated cluster energies from databases. In contrast to the method of cluster expansion, wMBE focuses on positional degrees of freedom and hence, explicitly handles structural relaxations during computations of stable atom clusters and periodic or amorphous phase structures. Integration of wMBE with cluster expansion methodology to address the problem of crystal structure prediction will be presented.

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