Valence Multipole Force Fields

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Typical molecular-scale potential energy models (force fields) use many-body decomposition to describe structural energy. Structural descriptors involving two or more bodies (e.g., interatomic distances, bond angles, out-of-plane bending angles, and torsional angles) are chosen, ideal values are selected for these descriptors, given different combinations of neighboring atoms, and functions are designed to describe the potential energy cost of deviations from these ideal values.

One persistent problem with standard force fields is that, in reality, there is no unique ideal value for structural descriptors like bond lengths or bond angles. Rather, they change in response to the total bonding environments of the atoms involved. To address this problem, we have developed a new type of force field, based on the valence multipole model (VMM) [1-4], which employs a multipole expansion of the bond valence incident to each atom.

In this presentation, we explain the basic architecture of this new type of potential energy model. VMM force fields separate the energy associated with each atom into terms related to total bonding (valence monopole), bonding asymmetry (valence dipole), and ellipsoidal deformation (valence quadrupole). All of these are inherently multi-body terms that are calculated by combining two-body terms (bond valences), reducing the computational cost. Ideal values of the structural descriptors are determined for different bonding scenarios, and energy cost functions for deviations are applied.

Initial results on the Al-Si-H-O system show that, provided bond valence sums are satisfied to within 0.2 v.u. of the ideal for all atoms, thermodynamic energies of equilibrium structures can be reproduced to within ~5 kJ/mol per unique atom. Development of the energy cost functions to reproduce far from equilibrium structures is ongoing. If this is accomplished, we will have a means of producing relatively accurate, reactive force fields with a minimal number of adjustable parameters.

[1] Shepherd *et al*. (2016) *Am. Min*., **101**, 362-370. [2] Wander *et al*. (2015) *Am. Min*., **100**, 160-171. [3] Wander *et al*. (2015) *Am. Min*., **100**, 148-159. [4] Bickmore *et al*. (2013) *Am. Min*., **98**, 340-349.