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A preliminary valence-multipole potential energy model: Al-Si-H-O system

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Abstract

Here we test the concept that a potential energy model (force field) based on an expansion of the bond-valence model can use molecular geometry to make a reasonable prediction of the thermodynamic energy. The backbone of the model is a non-standard choice of structural descriptors for the energy decomposition, which relates the energy to particular aspects of the structure. Most force fields use a many-body decomposition to describe structures (with two-, three-, and possibly four-body terms, etc.), whereas ours employs a multipole expansion of the bond valence incident to each atom. This valence multipole model separates 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). Provided bond valence sums are satisfied to within 0.2 v.u. of the ideal for all atoms, this model can provide accuracies of ~5 kJ/mol per unique atom in the Al-Si-H-O system, at least for the equilibrium structures tested here, comparable to most quantum mechanical calculations. More development is needed to produce a fully functional force field suitable for molecular dynamics simulations, but this work shows that the development of such a force field is likely to be feasible.

Keywords: Bond valence, multipole expansion, molecular mechanics, molecular modeling