

The Valence Multipole Model, issues with applying an energy model to Molecular Dynamics

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We have taken the valence multipole model (or VMM, an expanded version of the bond-valence model) and begun the process for implementing it into a molecular mechanics framework. The implementation is taking place as a user expansion module in the molecular modeling package, LAMMPS. This allows us to take advantage of the extensive capabilities of LAMMPS, including its modular structure. In time it should allow the VMM to function as a fully realized force field potential for MD simulation. The VMM has been shown to have a remarkable ability to correctly predict the energies of equilibrium structures, due to its ability to more correctly mimic the multi-body nature of chemical bonding.¹ However, this level of calibration is wholly inadequate to the level required for a full potential energy surface (PES). The requirement for an effective PES first requires recasting energies and gradients and then filling in the data into regions both near and far from equilibrium. This type of “data” is not realizable solely through experiment, which overwhelmingly favors equilibrium and near equilibrium configurations. Key to this problem is understanding the behavior of the “hard-sphere” repulsion terms that dominate away from equilibrium in a Bond Valence context. Given this need emphasis has shifted away from water as a primary liquid to understanding noble gas fluids that are far more simple, and understanding reached from these studies can be used to help fill in the missing pieces in our water force field. Preliminary simulations for liquid water and noble gas systems will be presented and their implementation issues discussed.

[1] Wander, Matthew & Barry Bickmore (Submitted 2015), *American Mineralogist*, "A preliminary valence-multipole force field: Al-Si-H-O system".