

Valence multipole molecular dynamics simulations of water

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We are developing molecular mechanics force fields based on a new way of conceptualizing molecular geometries—using a multipole expansion of the bond valence incident to each atom. Along with accompanying energy cost functions, this description is mathematically compact, easily incorporates multi-body interactions, and is capable of addressing reactions involving coordination number changes.

One of our main objectives is to use such force fields to simulate mineral-water interfacial chemistry, so it is important to test how well such a force field could be made to work on the aqueous phase. Therefore, we are testing a force field for the H-O system on liquid water, using molecular dynamics (MD) simulations.

Specifically, we are modifying the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) software package to handle the new force fields. Next, we will run MD simulations to see if the model can successfully predict the structure, dynamics, and thermochemistry of water. If it is successful, the model will use many fewer adjustable parameters than existing reactive force fields for water.