# A Novel, Computationally Efficient Multipolar Model Employing Distributed Charges for Molecular Dynamics Simulations



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A truncated multipole expansion can be re-expressed exactly using an appropriate arrangement of point charges. This means that groups of point charges that are shifted away from nuclear coordinates can be used to achieve accurate electrostatics for molecular systems. We introduce a multipolar electrostatic model formulated in this way for use in computationally efficient multipolar molecular dynamics simulations with well-defined forces and energy conservation in NVE (constant number-volume-energy) simulations. A framework is introduced to distribute torques arising from multipole moments throughout a molecule, and a refined fitting approach is suggested to obtain atomic multipole moments that are optimized for accuracy and numerical stability in a force field context. The formulation of the charge model is outlined as it has been implemented into CHARMM, with application to test systems involving H2O and chlorobenzene. As well as ease of implementation and computational efficiency, the approach can be used to provide snapshots for multipolar QM/MM calculations in QM/MM-MD studies and easily combined with a standard point-charge force field to allow mixed multipolar/point charge simulations of large systems.

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