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AMOEBA 2.0: A physics-first approach to biomolecular simulations JOSHUA RACKERS, JAY PONDER, Washington Univ — The goal of the AMOEBA force field project is to use classical physics to understand and predict the nature of interactions between biological molecules. While making significant advances over the past decade, the ultimate goal of predicting binding energies with "chemical accuracy" remains elusive. The primary source of this inaccuracy comes from the physics of how molecules interact at short range. For example, despite AMOEBA's advanced treatment of electrostatics, the force field dramatically overpredicts the electrostatic energy of DNA stacking interactions. AMOEBA 2.0 works to correct these errors by including simple, first principles physics-based terms to account for the quantum mechanical nature of these short-range molecular interactions. We have added a charge penetration term that considerably improves the description of electrostatic interactions at short range. We are reformulating the polarization term of AMOEBA in terms of basic physics assertions. And we are reevaluating the van der Waals term to match *ab initio* energy decompositions. These additions and changes promise to make AMOEBA more predictive. By including more physical detail of the important short-range interactions of biological molecules, we hope to move closer to the ultimate goal of true predictive power.

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