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An Empirical Charge Redistribution Model for Water Potentials in Biophysical Systems ROBIN SMITH, Swarthmore College, STEVE VALONE, Materials Science and Technology Division, Los Alamos National Laboratory, SUSAN ATLAS, Center for Advanced Studies and Department of Physics and Astronomy, University of New Mexico — Development of empirical atomistic models for simulations of biomolecules and biomaterials requires an understanding of charge transfer processes. Chemical potential equalization provides a conceptual basis for modeling electron redistribution during molecular conformational changes. A new charge-dependent energy formulation developed by Valone and Atlas extends current models based on CPE by permitting an accurate description of dynamic charge fluctuation during dissociation and charge transfer processes. We explore this formulation by constructing a conceptual submodel specific to the water molecule, important for understanding biophysical interactions in an aqueous environment.

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