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Charge-transfer water potential for solvated protein dynamics[1]
VIJAY JANARDHANAM, GODWIN AMO-KWAO, SUSAN R. ATLAS, Department of Physics and Astronomy, University of New Mexico — Water plays a critical role in simulations of complex structure-function relationships such as the mechanochemistry of molecular motor proteins, wherein solvating water molecules interact with divalent cations such as Mg^{+2}, salt bridges, and polar or charged amino acids. Existing fixed-charge and fluctuating charge water models are inadequate in these environments, since they do not support reactive charge transfer with proper long-range dissociation behavior. The charge-transfer embedded atom method (CT-EAM) potential of Valone and Atlas was developed to address these challenges. It includes charge-polarized and ionic embedding terms that describe many-body atomistic interactions as a statistical ensemble of integer-charge excitations; background embedding densities are functions of local pseudoatom electron density distributions that integrate to non-integer charges and evolve dynamically under chemical potential equalization. Here we report first results from simulations of water using the CT-EAM potential of [1] and compare with characteristic properties of the liquid as determined via conventional force fields. [1] K. Muralidharan, S. M. Valone, and S.R. Atlas. arXiv:cond-mat/0705.0857v1, submitted.

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