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A new lattice Monte-Carlo simulation for the dielectric inhomogeneity of ion-containing liquids XIAOZHENG DUAN, ISSEI NAKAMURA, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — We develop a novel lattice Monte-Carlo method to capture the effects of the reorganization of solvent dipoles under external electrostatic fields. Our simulation accounts for the effects of saturated dipoles near ions on the angstrom scale and hence spatial variations in the dielectric function. We will discuss the substantial disparity in the dielectric functions between like and unlike charges. Importantly, a contacting cation-anion pair cannot be literally taken as "charge-neutral species" in terms of the solvation energy. On the other hand, even when the two charges are separated by 1 [nm], a significant correlation in the dielectric function may arise. Our simulation also provides the dependence of the bulk dielectric value on the ionic strength, which is consistent with experimental data.

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