Abstract Submitted
for the SES11 Meeting of
The American Physical Society

Image Charge Optimization for the Reaction Field by Matching to an Electrostatic Force Tensor WEI SONG, DONALD JACOBS — A new image charge solvation model has recently been developed, which consists of a spherical cavity of explicit solvent embedded in a continuum dielectric medium. Inside the cavity, the dielectric constant is 1 and outside the cavity is set to 80. Although the discontinuity from 1 to 80 at the cavity interface creates large artifacts near the boundary, MD simulation using this model yields accurate results by incorporating a buffer layer containing imaged water. We generalized the model to reflect a continuously changing dielectric profile at the boundary, and optimized image charges for the reaction field based on electrostatic forces to minimize the buffer layer volume and reproduce the electrostatic force field associated with the dielectric properties of the model solvent. However, MD simulation suggests that the new model is unstable. Previously, we also showed that the reaction field has an order of magnitude stronger influence on the electrostatic torque compared to force on solvent water molecules. Therefore, we optimize the image charges in a different way, using a force tensor defined by a grid of dipoles, which places more constraints on the system.

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Date submitted: 24 Aug 2011 Electronic form version 1.4