

Abstract Submitted
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Implementation of the Surface Charge Method for Calculation of Biomolecular Electrostatic Forces¹ T. P. DOERR, Y.-K. YU, National Center for Biotechnology Information, NIH — Due to the presence of ions, a high dielectric constant solvent (water with $\epsilon = 80$), and significant charges and polarizabilities associated with many biomolecules, electrostatic forces play a crucial role in biomolecular interactions. It is particularly important to account for the effects of the solvent. The surface charge method (SCM), developed in PRE **73**, 061902 (2006) can be applied straightforwardly to a system of an arbitrary number of charged dielectric spheres embedded in an infinite dielectric solvent. Although in principle the electrostatic energy and force can be calculated to any desired accuracy using the SCM by simply including more multipole moments in the expansions, in practice this process leads to large matrix inversions that are inefficient to carry out. Therefore it was necessary to derive a scheme so that higher order multipole moments could be incorporated into the description of the system without leading to unacceptably large matrix inversions. We have implemented such a scheme and applied it to a system of such spheres in a solvent and explored the effect in this system of asymmetric dielectric screening, which was revealed during the development of the SCM.

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