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Surface Charge Method Calculation of Biomolecular Electrostatic Force with Application to a Model System[1] TIMOTHY DOERR, YI-KUO YU, National Center for Biotechnology Information, NLM, NIH — Due to the presence of ions, a high dielectric constant solvent (water with $\varepsilon = 80$), and significant charges and polarizabilities associated with many biomolecules, electrostatic forces play a crucial role in biomolecular interactions. It is particularly important to adequately account for the effects of the solvent. The surface charge method presented here has been applied to a system of an arbitrary number of charged dielectric spheres embedded in an infinite dielectric medium (the solvent). The surface charge method allows calculation (to any accuracy desired) of the energy and the various forces using only matrix inversion. The energy and forces are relatively insensitive to the value chosen for the dielectric constant inside the spheres. For the special case of two isolated charged dielectric spheres in an infinite medium, the results are not obvious: The repulsive force for like-charged spheres is strengthened (compared to point charges in the solvent medium) at short distances, while the attractive force for oppositely-charged spheres is to a lesser degree weakened at short distances. In the limit that the charges associated with a biomolecule are point-like, the excess repulsion and suppressed attraction found here might play a role in minimizing the effect of energetic traps.

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