160b Solvation Study Using Gaussian Charges Particles and GCPM Water Model

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The solvation of charge ions in water is an important process due to its ubiquity in nature and engineered chemical and biological systems. Solvation studies using molecular simulation methods abound in the published literature (for example, see Refs. [1,2]); however, almost all of these simulation studies have featured models for the water and for the ions that, in terms of electrostatic interactions, consist of non-polarizable point charge models. In the simulations reported here, in order to obtain a more accurate description of solvation processes, we have used a polarizable model for ion with a Gaussian charge. We have focused on the effect of varying of the charge, size and degree of smearing of the ion on the solvation energy.

We modeled the water solvent using a recently developed polarizable water model containing Gaussian charges (GCPM) [3], which satisfies the water monomer and dimer properties and accurately predicts the dielectric, structural and vapor-liquid equilibria and transport properties of water over the entire fluid range.

REFERENCES

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