SYSTEMATIC INVESTIGATION OF ELECTROSTATIC AND CORRELATION EFFECTS IN WATER CLUSTER ANIONS

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Recent investigations have found that there is a link between the balance of electrostatic and correlation effects present and the morphology of water cluster anions. However, using *ab initio* methods it is somewhat difficult to separate out the type and magnitude of these interactions. Using a Drude-type model first introduced by Jordan *et al.* [a] a systematic investigation is made into the effect of both the size and type of multipole expansion used to represent the charge distribution on the water molecules making up the cluster, the effect of polarization, and electron correlation. This will elucidate how the different interactions affect the geometry of the water cluster, particularly with regard to the issue of cavity vs. surface states. The results from the model will be compared with previous *ab initio* calculations.

[a] F. Wang and K. D. Jordan *J. Chem. Phys.* **114**, 10717 (2001)