The Supplementary Materials for

Fragment Quantum Mechanical Method for Large-sized Ion-water Clusters

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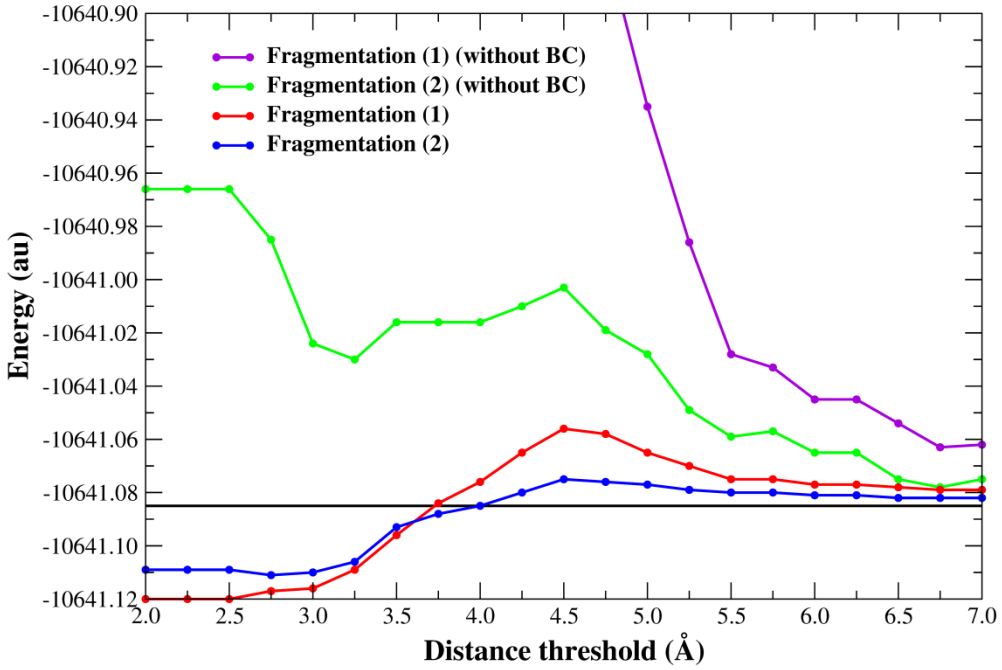

Figure S1. The total EE-GMF energy of the water cluster (140 water molecules) as a function of the distance threshold λ_2 for three-body interactions. The distance threshold for two-body interactions was fixed at λ_1=7.0 Å. "Fragmentation (1) (without BC)" sets one water molecule as a fragment without the presence of the background charges of the environment in each fragment QM calculation. "Fragmentation (2) (without BC) uses two nearest water molecules as a fragment without the presence of the background charges of the environment in each fragment QM calculation. On the other hand, "Fragmentation (1)" and "Fragmentation (2)" utilize the electrostatic embedding scheme in each fragment QM calculation. The total energy from the full system calculation (black line) is regarded as the reference.