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The role of non-additive contributions on the hydration shell structure of Mg^{2+} studied by Born–Oppenheimer ab initio quantum mechanical/molecular mechanical molecular dynamics simulation

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Abstract

An ab initio quantum mechanical/molecular mechanical (QM/MM) molecular dynamics simulation has been performed to investigate the effects of non-additive contributions on the hydration shell structure of Mg^{2+}. The active-site region, the sphere including the second hydration shell of Mg^{2+}, was treated by Born–Oppenheimer ab initio quantum mechanics, while the rest is described by classical pair potentials. A hydration complex with six inner shell waters and 12 second shell waters was observed. It was also found that the effects of non-additive terms play an important role in the preferential orientation of water molecules inside the hydration sphere of Mg^{2+}. © 2001 Published by Elsevier Science B.V.