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Structural arrangement and dynamics of the hydrated Mg^{2+}: An ab initio QM/MM molecular dynamics simulation

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Abstract

The structural arrangement and dynamics of solvated Mg^{2+} in dilute aqueous solution have been studied by ab initio QM/MM molecular dynamics simulation, in which the whole first and most of the second hydration shell of the ion were treated at Hartree–Fock level using LANL2DZ basis sets. Besides the most stable $Mg^{2+}(H_2O)_6$ species, intermediates such as $Mg^{2+}(H_2O)_5(H_2O)$, where at least one water molecule temporarily moves into the inter-shell region but remains H-bonded to inner-shell water, as well as transition complexes of the $Mg^{2+}(H_2O)_6(H_2O)$ type, exist in aqueous solution. The dynamics of solvate and surrounding water molecules are discussed in connection to the 'structure-forming' ability of Mg^{2+}.