

Hydration of a coarse-grained methyl-ion solute

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Studies investigating the properties of Hg-containing molecular species in aqueous environments are essential to understanding the mechanism of food chain contamination. In order to provide new insight into the cellular uptake of Hg species, we are developing a coarse-grained model of a simple methyl-ion model with the goal of uncovering information regarding the behavior of toxic methylmercury in aqueous media. While there is much research studying the solute-solvent interactions of either an ion or a nonpolar molecule in water, we are using molecular dynamics to study a bonded pair of two particles, one representing a very hydrophilic ion-like particle without charge while the other is a hydrophobic methane-like particle. The hydration of this methyl-ion pair is compared to aqueous systems of coarse-grained ionic solutes representing varying size and charge.