Multi-length scale modeling applied to alkali metal ions in liquid water

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In aqueous media, interactions between ions and water lead to local deviations from the bulk water density. These structural changes in water affect simple transport of the ions as well as selective transport, where interactions between ions and the substrate help determine which ions are restricted from passage through a pore, for example. Using ab initio molecular dynamics in tandem with classical density functional theory, we study the structural changes in water induced by alkali metal ions and relate them to the predicted differences in thermophysical properties of the ions. Comparisons with experimental data show the strength of this approach.