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Microsolvation of lithium iodide dimer studied by *ab initio* calculations

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Abstract

The structures of microsolvated $(\text{LiI})_2^-(\text{H}_2\text{O})_n$ ($n = 0-6$) clusters and their corresponding neutrals were determined using *ab initio* calculations. One Li-I distance in $(\text{LiI})_2^-(\text{H}_2\text{O})_n$ abruptly increases at $n = 5$, thus a I atom is firstly separated out from the $(\text{LiI})_2^-$ unit. For the neutrals, the notable elongation of Li-I distances occurs at $n = 4$, and a I atom prefer to leave the $(\text{LiI})_2$ unit. The charge analyses show that the excess electrons mainly localizes on the terminal Li atom for $(\text{LiI})_2^-(\text{H}_2\text{O})_{0-1}$, whereas charge transfer to water occurs when the number of water reaches 2. The RDG analyses show that Li^+ -water interactions are dominant, and with the increase of water molecules, the I^- -water and water-water interactions are considerably enhanced. The comparison of $(\text{LiI})_2^-(\text{H}_2\text{O})_n$ and $(\text{MI})_2^-(\text{H}_2\text{O})_n$ ($\text{M}=\text{Na}, \text{K}$) indicates that $(\text{LiI})_2^-$ is more difficult to be pried apart than $(\text{MI})_2^-$.

Keywords: LiI-water cluster; structural evolutions; microsolvation; charge transfer; interaction analyses

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