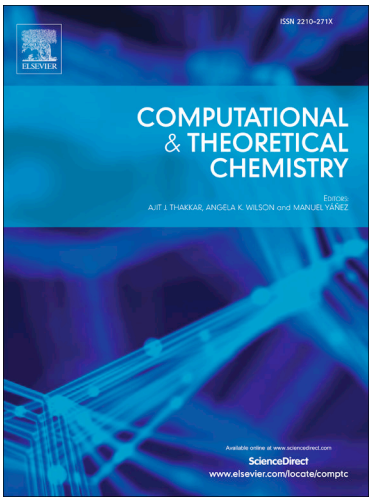

Microsolvation of lithium iodide dimer studied by *ab initio* calculations

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

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Abstract

The structures of microsolvated $(LiI)_2^-(H_2O)_n$ (n = 0-6) clusters and their corresponding neutrals were determined using ab initio calculations. One Li-I distance in $(LiI)_2^-(H_2O)_n$ abruptly increases at n = 5, thus a I atom is firstly seperated out from the $(LiI)_2^-$ unit. For the neutrals, the notable elongation of Li-I distances occurs at n = 4, and a I atom prefer to leave the $(LiI)_2$ unit. The charge analyses show that the excess electrons mainly localizes on the terminal Li atom for $(LiI)_2^-(H_2O)_{0-1}$, 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 $(LiI)_2^-(H_2O)_n$ and $(MI)_2^-(H_2O)_n$ (M=Na, K) indicates that $(LiI)_2^-$ is more difficult to be pried apart than $(MI)_2^-$.

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