Title: Li+−Li+ and Na+−Li+ ion pairs in aqueous solution

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Abstract: Like ion pair Li+−Li+ and mix ion pair Na+−Li+ in aqueous solution were investigated by high level ab initio calculation and quantum mechanical effective fragment potential molecular dynamics (QM/EFP MD). Our QM/EFP-MD predicts that like ion pair Li+−Li+ are more likely to be observed than mix ion pair Na+−Li+ in the solution. In a particular, the formation of Li+−Li+ is less than that of Na+−Na+, and the formation of Na+−Li+ is even worse. The local structural analysis indicates that three-water bridging structure is dominating in Li+−Li+ion pair in the solution whereas the Na+−Li+ ion pair mostly bound to one water molecule. Both the MD and QM study suggests that one water bridging structure is very unstable.

Keywords: Ion pairing, Li^+–Li^+ ion pair, Na^+–Li^+ mixed ion pair, Ab initio calculations

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