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**A microscopic view of ion solvation in aqueous and non-aqueous electrolyte solutions from molecular dynamics simulations**

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**Abstract**

Molecular dynamics simulations were performed to understand the ionic association and its effect on the structure and dynamics of ion solvation shell in aqueous and non-aqueous electrolyte solutions (water and methanol). The simulation results show that the probability of ion pairing depends on the interplay between ion-solvent interactions on the one hand, and Coulomb forces between ion and its counter-ion on the other hand. The highest probability of ion-pairing is observed for LiF due to the strong Columbic attraction between Li<sup>+</sup> and F<sup>-</sup> ions. This is evident from the calculated radial distribution functions and orientation of solvent molecules which show signatures of ionic association in water and methanol. Due to low dielectric constant of methanol, the probability of ionic association is higher in methanol than water and the probability of ionic association decreases with increasing size of ion or counter-ion. The coordination number and mean residence time is found to be influenced by the inter-ionic attraction. Detailed analysis of Potential of Mean Force (PMFs) and Mean Residence Time (MRT) of solvent molecules reveal how the stability of ionic solvation shell is influenced by the inter-ionic attraction and other properties of the solvent.

**Keywords:** MD simulation, ionic association, mean residence time, ion solvation, potential of mean force

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