

Adsorption of Ions at Solid-Liquid Interface: Role of Ion Hydration Structure and Energies

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The adsorption of ions on charged surface creates distribution of counter- and co-ions from surface to the bulk region, which is referred to as electrical double layer (EDL). In EDL, some of the ions are in direct association with the surface while rest of the ions are distributed away from the surface till bulk region. The recently developed super-capacitors^{1,2} physically store high density charge in terms of these EDL at the electrode surface. In addition, ion adsorptions at solid-liquid interface play crucial role in remediation of heavy metal ions, water purification by ion-exchange, minerals formation and surface catalytic reactions.

The adsorption of ions at the solid-liquid interface is governed by their distribution, hydration structure and hydration energies. Here, we have performed molecular dynamics simulation studies of monovalent (Na^+ and Rb^+) and divalent (Mg^{2+} and Sr^{2+}) ions at various concentrations at mica surface. These ions have varying hydration energies and hydration structure, and our simulation studies cover wide ranges of concentrations. Since, divalent ions have higher hydration energies, we expected their adsorption to be higher compared to monovalent ions having lesser hydration energies. However, we observed counter-intuitive behaviour of higher monovalent adsorption at all concentrations. We have analysed the potential of mean force of these ions, their coverage and hydration structure near mica surface to explain these observed behaviors.³

References:

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