

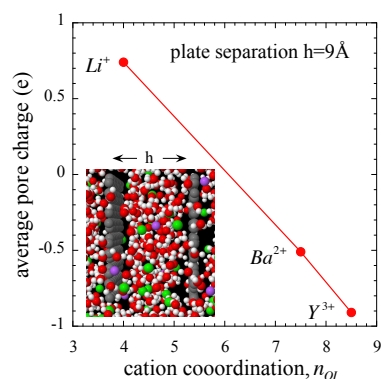
Interfacial and confined behavior of water and aqueous electrolytes between finite graphene plates

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Achievement

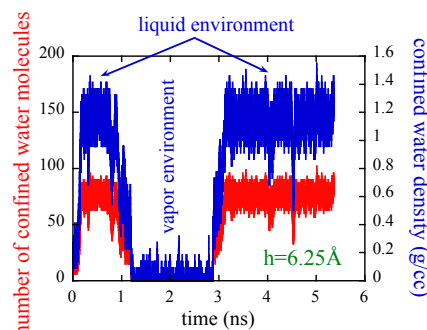
We have shown how, at global isobaric-isothermal conditions, the interplay between confinement and ionic differential hydration behavior, *i.e.*, significant differences of hydration numbers, would prevent local electroneutrality through the selective expulsion from the confined spaces of ions bearing larger hydration shells. Our molecular dynamics results suggest that hydrated ions would rather move away from confined environments than shave their hydration shells. Moreover, due to the pronounced reduction of the hydrogen bonding at the water-graphene plate interfaces, the confined water becomes unstable, and it is gradually expelled from the confined space following a de-wetting process typically expected for hydrophobic water-plate interactions. This instability translates into an oscillatory density transition between vapor and liquid phases in contact with the graphene plates at an inter-plate separation of $\sim 6.25\text{\AA}$.



Dependence of the average pore charge on the cation's water coordination n_{O_l}

Significance

Molecular-based interrogation of the confinement behavior of aqueous electrolytes, resulting from the overlapping of interfacial regions, provides a powerful tool for the understanding of the link between the species hydration, the extent of fluid confinement, and the nature of the solid-fluid interactions. Acquiring this knowledge becomes crucial for the manipulation, and ultimately, the control of local electrochemical properties at a molecular level for specific energy-related applications.



Wet/dry transition in confined water between finite graphene plates at ambient conditions for $h = 6.25\text{\AA}$

Credit

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