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Solvation of ions in bulk and at interfaces: What can density functional theory teach us?[1]

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Insights from molecular simulation have influenced both experiment and theory regarding the understanding of the specific ion effect. Although there seems to be a consensus that large polarizable anions exist at the air-water interface, the understanding of the precise molecular interactions that give rise to surface adsorption remain elusive. I will present our work on the adsorption of iodide at the air-water interface using density functional theory (DFT) based interaction potentials. I will discuss similarities and differences of the results obtained using different descriptions of molecular interaction. Last, we are able to reconcile the results obtained with molecular simulation using standard empirical potentials with the dielectric continuum theory of Levin and co-workers.

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