Electrostatic Origin of Element Selectivity during Rare Earth Adsorption

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Lanthanides are rare earths used in high-tech applications, in medicine, and in biology. They are often extracted from aqueous solutions using surfactants at oil-water interfaces. Despite decades of research, there is very little understanding of fundamental aspects of this process.

Using x-ray fluorescence measurements and theoretical arguments, our study indicates that the known strong dependence of lanthanide extraction efficiency on atomic number originates at the surfactant interface, rather than in the bulk or in dynamic effects during the extraction process. We expect that a better understanding of the basic physics of these systems will help improve the methods and materials used in these commercially important processes.

(a) Schematic diagram of the system being simulated. (b) Sample Monte Carlo simulation setup (smaller $20 \times 20$ system shown here for clarity) in the model of two sharp interfaces separated by distance $d_{\text{inter}}$. The upper interface is in contact with air and the lower interface is in contact with water. The upper hexagonal lattice layer is the molecular monolayer and the lower hexagonal lattice layer is composed of lanthanides. Red indicates charged molecules, blue is absorbed lanthanides, and white is neutral molecules (upper layer) or empty lanthanide sites (lower layer). The separation in the $z$ direction ($d_{\text{inter}}$) is exaggerated here for clarity.