

The Role of Cation Solvation Thermodynamics in Surface Complexation Reactions

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Previous studies of cation exchange and adsorption at solid-water interfaces from this and other groups have highlighted the role of solvation properties and thermodynamics of ions and surface species in governing how these fundamental reactions unfold. Specifically, solvation and desolvation energies were reported to influence the partitioning of cations between inner- and outer-sphere species and determine, at least qualitatively, the net sign of the reaction enthalpy. Variables that change the local solvation structure and ion (de)solvation energy cost, e.g., nanoconfinement and hydrolysis, impact the cation coordination environment and bonding to the solid's surface. Herein, we will report on new experimental and computational findings for cation exchange reactions and analyze observed trends as they relate to a number of solids including rutile, quartz, zeolites, nanoporous silica, and Mxenes. A broader discussion on how to compile the current collection of *ad hoc* interpretations into a unified formalism concerning the thermodynamics of chemical interfacial reactions will be included.

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