

The thermodynamics of halide exchange at oxide-aqueous solution interfaces from microcalorimetry and modeling experiments

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Previous thermodynamics studies of ion exchange and adsorption at metal oxides-aqueous solution interfaces from this group (among others) have predominantly focused on cations. These studies highlighted the role that hydration properties play in governing the thermodynamics of complexation reactions. Less studied are anions despite a general recognition that their presence, as background electrolyte, could also be influential. Herein, we examine the thermodynamics of a suite of monovalent halide ions (F, Cl, Br, I, and NO₃) interacting with nanoparticles of hematite and anatase. Using flow microcalorimetry to measure the in situ and operando enthalpies of anion adsorption and exchange, we will summarize chemical trends by probing the effect of size, solvation enthalpies (DH_{solv}), and speciation on the sign and size of the observed energetics. These data will be augmented with modeling efforts to further our understanding of the role these anions play in interfacial chemistry. The implication of these results for our understanding of ion exchange as a basis for contaminant transport, mineral dissolution and precipitation, etc. will be also be presented.