U(VI) desorption from capillary fringe sediments

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U (VI) contaminated capillary fringe sediments at Hanford 300 Area are considered to secondary source for existing uranium plume in groundwater. Because seasonal water table elevation and water chemistry changed in response to nearby Columbia River stage, batch and column desorption experiments of U (VI) were conducted using two U (VI) contaminated sediments (11D and 39B).

Solid phase characterization of these two sediments was performed to identify mineralogic and chemical factors controlling U (VI) desorption. The desorption behavior of U (VI) was different from the two sediments in spite of similar chemical and textural characteristics. Adsorption strength and sorbed U (VI) lability was higher in the near-river sediment, 11D. Inland sediment, 39B displayed low sorbed U (VI) lability (~10%) and measurable solid-phase carboante content. Kinetic desorption was attributed to regeneration of labile U (VI) in 11D.

The U (VI) desorption reaction was best described as an equilibrium surface complexation reaction. The noted differences in U (VI) desorption behavior appear to result from U (VI) contamination and hydrologic history, as well as sediment carbonate content.

First-principles investigation of order-disorder phase boundary in ice

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Ice has a very rich phase diagram. Up to now, sixteen crystalline phases have been identified experimentally. This richness of the phase diagram originates in part in hydrogen order-disorder (OD) transitions. The ice VII-VIII boundary, a typical OD boundary, has been reasonably well constrained experimentally and is an ideal study case. We present a first-principles quasiharmonic study consisting in the complete statistical sampling of molecular orientations within a 16 molecule supercell. This supercell calculation accounts for several aspects of this transition, including the Clapeyron slope and the isotope effect. Research suppported by NSF grants ATM 0428874 (VLab) and EAR 0757903. Computations were performed at the Minnesota Supercomputing Institute.