Glenn T. Seaborg Center Seminar

Modeling uranyl complexation by humic substances and adsorption on solvated clay mineral surfaces

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4:00 – 5:00 pm
Perseverence Hall - Bldg. 54 Room 130

Using density functional methods, the seminar reports computational studies of two timely issues in actinide chemistry: (i) actinide complexation by natural organic matter and (ii) adsorption of actinides on clay minerals. Both topics are of major concern for the distribution and the transport of actinide ions in the environment.

To explore the complexation propensity of humic substances with uranyl (VI), organic molecules were chosen as models of various functional groups. Complexes of uranyl with model ligands were studied in solution applying an all-electron relativistic density functional approach. Besides carboxylic functional groups which have been assumed to play a major role in uranyl complexation, also aliphatic and phenolic OH, as well as sulfonate and nitrogen-containing groups were studied.

Uranyl adsorption on bare and solvated kaolinite surfaces was explored by density functional calculations on periodic slab models. Surface solvation was approximated by a monolayer of water molecules. For kaolinite, outer- and inner-sphere surface complexes on (001) basal and (010) edge surfaces were an extensively surveyed. Our findings suggest an extension of the current interpretation of pertinent EXAFS and TRLFS experiments.

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