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Titel des Beitrags: Density Functional Model Study of Uranyl Adsorption on the Solvated (001) Surface of Kaolinite

Abstract: We studied the adsorption of uranyl on bare and solvated models of the octahedral (001) surface of kaolinite using first-principles density functional calculations. Inner-sphere bidentate complexes adsorbed at partially deprotonated short-bridge sites AlOO(H) and long-bridge sites AlO-AlO(H) were modeled as the most probable adsorption complexes. The uranyl complex at the doubly deprotonated AlO-AlO long-bridge site exhibits a third contact to the surface, not present in the complex at the corresponding short-bridge site. Adsorption at short-bridge sites is energetically favored compared to complexes at long-bridge sites. We were unable to determine stable adsorption complexes of uranyl at singly deprotonated AlO-AlOH long-bridge sites. Surface solvation, approximated via an adsorbed monolayer of water molecules, hardly affects the adsorption complexes of uranyl. Contacts U-O(eq) in the equatorial plane shorten by 2 pm, U-Al distances elongate by up to 4 pm. In contrast to the bare surface, adsorption complexes at long-bridge and short-bridge sites of the solvated surface exhibit similar stabilities.

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