We report density functional investigations of kaolinite edge surfaces and uranyl adsorption thereon. Applying periodic slab models, we studied the (0 1 0) surface of kaolinite as an example of kaolinite edge facets which are expected to be highly reactive and to adsorb preferentially metal ions. Among the four terminations of the (0 1 0) surface, we selected the two most likely ones and determined their structures to be affected by solvation. On these modified surfaces, we explored bidentate inner-sphere adsorption complexes of uranyl, at single metal center sites, Al(O,OH), and sites of mixed type, AlOH-SiO. On one of the terminations hydrolysis of uranyl was found to occur. Comparison of key calculated structure parameters with available experimental data suggests an extension of the prevailing interpretation and implies that a set of uranyl complexes may coexist on edge surfaces. (C) 2010 Elsevier Ltd. All rights reserved.
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