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Density Functional Theory Studies of Sb(V) Oxyanion Adsorption on α-Al_2O_3 $1\bar{1}02$ surfaces SAI KUMAR RAMADUGU, SARA MASON, University of Iowa — We apply density functional theory and periodic slab models to understand the adsorption and reactivity of $Sb(OH)_6^{-1}$ on various surface terminations of α-Al_2O_3 $(1\bar{1}02)$. On all surfaces studied, Sb(V) adsorption is preferred when adsorbed in a bidentate, corner-sharing geometry. On the other hand, all theoretical bidentate edge-sharing modes are relatively high in energy. This is in good agreement with recent experiments that do not observe any bidentate edge-sharing adsorption of $Sb(OH)_6^{-1}$ on hydrous aluminum oxide. We identify factors that govern the preference for corner-sharing adsorption, and compare how well the surface reactivity can be predicted based on periodic DFT *vs.* quantum chemical cluster models. From the DFT projected density of states, we clearly show how strained ligands of Sb(V) cannot achieve good overlap with the electronic states of the surface, even at Sb-O distances predicted to be ideal by empirical bond-valence. The results thus provide a molecular-level understanding of Sb(V) specific adsorption and also allow us to assess other modeling approaches to computational geochemical surface science.

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