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[◀ Prev Article](#)**Abstract****Sulphate adsorption at the Fe (hydr)oxide-H₂O
interface: comparison of cluster and periodic slab
DFT predictions**K. W. PAUL^a, J. D. KUBICKI^b & D. L. SPARKS^a

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 K. W. Paul. E-mail: kpaul@udel.edu**Summary**

The transport and bioavailability of sulphate in soils are significantly affected by adsorption reactions at the mineral-H₂O interface. Therefore, an understanding of the mechanisms and kinetics of sulphate adsorption is of fundamental importance in soil chemistry. In this investigation, the binding geometries of bidentate bridging and monodentate sulphate complexes at the Fe (hydr)oxide-H₂O interface were predicted with static cluster and periodic slab density functional theory (DFT) calculations. The cluster calculations were performed with edge-sharing dioctahedral Fe³⁺ models, using the unrestricted PBE0 exchange-correlation functional and a combination of effective core potential (LanL2DZ - Fe atoms) and all-electron (6-311+G(d,p) or 6-311+G(3df,p) - S, O, and H atoms) basis sets. The periodic slab calculations were performed with a (3 × 2) slab of the (100) α-FeOOH surface, by means of the projector-augmented wave method and a plane-wave basis set. For the periodic slab DFT calculations, the spin-

polarized (SP) PBE exchange-correlation functional, with and without explicit consideration of an on-site Coulomb interaction parameter (i.e. SP-PBE and SP-PBE+U methods), was used. Despite the lack of long-range order, cluster model predictions of the interatomic distances and angles of bidentate bridging and monodentate sulphate were in good agreement with the periodic slab model predictions. Quantitative analysis of the cluster and periodic slab DFT predictions is expected to result from theoretical fitting of extended X-ray absorption fine structure measurements. The application of computational chemistry methods to soil chemistry research is anticipated to provide novel insight into the mechanisms and kinetics of ion sorption.

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