

University of Delaware User name: Password:

GO 🜔

Register Forgotten Password Athens/Institution Login

Synergy Home | Browse | Search | My Synergy | Books Online | Resources | About | Help



#### Journal Menu

Home > List of Issues > Table of Contents > Article Abstract

# Table of Contents

List of Issues

### Tools

- Email this article
- Add to favorite articles
- Export this citation
  Alert me when this article is cited: Email | RSS

# **Publication history**

(What is this?)

#### Published article online: 22 Jun 2007 Issue online: 18 Jul 2007

Received 24 February 2007; revised version accepted 14 May 2007

# European Journal of Soil

# Science

Volume 58 Issue 4 Page 932-944, August 2007

**To cite this article:** J. D. KUBICKI, K. D. KWON, K. W. PAUL, D. L. SPARKS (2007) Surface complex structures modelled with quantum chemical calculations: carbonate, phosphate, sulphate, arsenate and arsenite European Journal of Soil Science 58 (4), 932–944. doi:10.1111/j.1365-2389.2007.00931.x

## 4 Prev Article | Next Article 🕨

## Abstract

# Surface complex structures modelled with quantum chemical calculations: carbonate, phosphate, sulphate, arsenate and arsenite

J. D. KUBICKI<sup>a</sup>, K. D. KWON<sup>a</sup>, K. W. PAUL<sup>b</sup> & D. L. SPARKS<sup>b</sup>

<sup>a</sup>The Pennsylvania State University, Department of Geosciences and the Earth and Environmental Systems Institute, University Park, PA

16802, and <sup>b</sup>University of Delaware, Department of Plant and Soil Sciences, Newark, DE 1971,7 USA

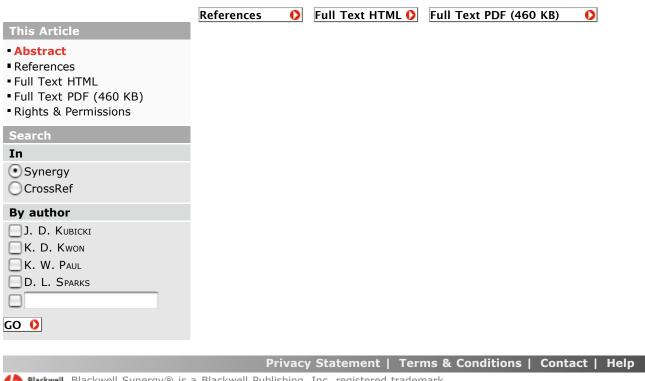
J. Kubicki. E-mail: <u>kubicki@geosc.psu.edu</u>

## Summary

Hybrid molecular orbital/density functional theory (MO/DFT) calculations on molecular clusters were used to model infrared (IR) vibrational frequencies and interatomic distances obtained via extended X-ray absorption fine structure (EXAFS) spectroscopy. Molecular clusters were found to provide good agreement with experimental observations for the oxyanions carbonate, phosphate, sulphate, arsenate and arsenite. The results show a consistent tendency to form bidentate bridging surface complexes at low pH, but the protonation and hydration states play a significant role in the results obtained from calculation as various protonation states of monodentate surface complexes are also predicted to be stable

as pH increases (i.e. the number of H<sup>+</sup> ions in the model are decreased). A method for estimating the Gibbs free energy of adsorption ( $\Delta G_{ads}$ ) is discussed to complement the comparisons of experimental and theoretical spectroscopic parameters. Calculated  $\Delta G_{ads}$  values were consistent with the interpretations based on

modelling observed spectra.



Blackwell Blackwell Synergy® is a Blackwell Publishing, Inc. registered trademark Publishing Partner of CrossRef, COUNTER, AGORA, HINARI and OARE

Technology Partner — <u>Atypon Systems, Inc.</u>