

## Density functional theory study of the interaction of arsenic complexes with FeOOH surfaces

KATRIN OTTE\*, WOLFGANG W. SCHMAHL  
AND ROSSITZA PENTCHEVA

Department of Earth and Environmental Sciences, University of Munich, Theresienstr. 41, 80333 Munich, Germany  
(\*correspondence: Katrin.Otte@lrz.uni-muenchen.de, Pentcheva@lrz.uni-muenchen.de )

Iron oxyhydroxides (FeOOH) possess high surface areas which are relevant for cycling and retention in a series of environmental and technological processes [1]. Using density functional theory (DFT), we explore the stability and electronic properties of the goethite (101), akaganeite (100), and lepidocrocite (010) surfaces under different environmental conditions. The GGA+*U* calculations reveal that the termination impacts the oxidation state of the surface iron ions, providing a possibility to tune the catalytic activity. The energetics and bonding mechanisms of arsenic complexes in different adsorption geometries (e.g. mono- and bidentate) on the surfaces are investigated.

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[1] R. M. Cornell & U. Schwertmann, *The Iron Oxides* (Wiley, Weinheim, 2001).

## Quantification of primary marine organic aerosol properties using aerosol mass spectrometry

J. OVADNEVAITE<sup>1\*</sup>, D. CEBURNIS<sup>1</sup>, H. BERRESHEIM<sup>1</sup>,  
M. DALL'OSTO<sup>1,2</sup>, J. BIALEK<sup>1</sup>, C. MONAHAN<sup>1</sup>,  
D.R. WORSNOP<sup>3,4</sup> AND C.D. O'DOWD<sup>1</sup>

<sup>1</sup>School of Physics and Center for Climate and Air Pollution Studies, Ryan Institute, National University of Ireland Galway, Galway, Ireland

(\*correspondence: jurgita.ovadnevaite@nuigalway.ie )

<sup>2</sup>Institute of Environmental Assessment and Water Research, Consejo Superior de Investigaciones Científicas, Barcelona, Spain

<sup>3</sup>Aerodyne Research, Inc., Billerica, Massachusetts, USA

<sup>4</sup>Physics Department, University of Helsinki, Helsinki, Finland

Marine aerosol has a strong impact on both the Earth's albedo and climate; however, its inherently complex composition ranging from inorganic components (sea salt, nss sulfate) to complex organic carbon mixtures of water soluble and insoluble components [1, 2] and bio - aerosol components [3] complicates the quantification of those impacts. In recent years, the dominant organic matter (OM) contribution (in particular, the primary organic matter) to submicron marine aerosol during periods of high biological activity over N.E. Atlantic has been quantified on a seasonal basis [1] as well as in real-time [4]. However, the character of its influence on cloud formation is still undergoing an intense discussion. Here, we present the comprehensive long term real time ambient aerosol measurements which reveal the important role of marine organics to cloud formation: the recurrent enhancement of cloud formation activity (cloud condensation nuclei) under aerosol enrichment by primary organics with low hygroscopic growth factor is reported for the first time. Moreover, the complexity of organic matter identified by high resolution time of flight aerosol mass spectrometry (HR-ToF-AMS) and its interpretation from HR-PMF (Positive matrix factorization) revealed a dominant contribution of primary sources to marine organic aerosol, with unique marine organic aerosol fingerprint, when compared to anthropogenic organic aerosol.

[1] O'Dowd, C.D. *et al.* (2004) *Nature* **431**, 676-680.

[2] Russell, L.M. *et al.* (2010) *P. Natl. Acad. Sci. USA* **107**(15) 6652-6657. [3] Leck, C. & E.K. Bigg (2005) *Geophys. Res. Lett.* **32**(19) L19803. [4] Ovadnevaite, J. *et al.* (2011)

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