

Combining In situ Infrared Spectroscopy and DFT Theoretical Studies to Reveal the Structure of Adsorbed Metal Complexes

G. LEFEVRE*, A. DAVANTES, D. COSTA

PSL Research University, Chimie ParisTech — CNRS,
Institut de Recherche de Chimie Paris, 75005, Paris,
France (*correspondence: gregory.lefevre@chimie-paristech.fr)

The reactivity of inorganic material surfaces has many applications, and particularly in environment for the control and prediction of the migration of pollutants in soils and groundwater. Informations about structure of the surface species are needed for a better understanding and modelling of the adsorption mechanisms.

For several years, we have developed an approach based on in situ and real time analysis of surface complexes using Attenuated Total Reflectance - infrared spectroscopy. This technique allows us to get IR spectra of adsorbed species without any preparation of samples which could modify the surface speciation. This approach was successfully used to reveal the structure of (poly)molybdate and (poly)tungstates adsorbed on ferric (hydr)oxides [1-3]. We showed that, the structure of the adsorbed species differ with the nature of the iron (hydr)oxide in contact with the solution, from inner-sphere complexes to surface polymers. DFT calculations and experiments using of polarized ATR-IR setup have allowed us to interpret in situ spectra, and to deduce the structure of the surface species.

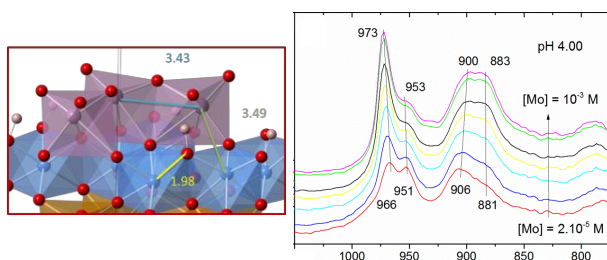


Figure 1: Surface polymerization of molybdate ions on hematite surface

[1] A. Davantès, D. Costa, G. Lefèvre (2016) J. Phys. Chem. C 120, 11871-11881. [2] A. Davantès, G. Lefèvre (2016) Surf. Sci. 653, L88-L91. [3] A. Davantès, D. Costa, B. Sallman, S. Rakshit and G. Lefèvre (2017) J. Phys. Chem. C 121, 324-332