

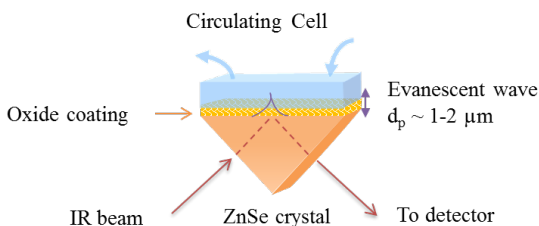
# (Poly)molybdate and (poly)tungstate ions sorption onto iron (Hydr)oxide: A combined *in situ* ATR-FTIR/DFT study

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The reactivity of the inorganic material surface has many applications and particularly in environment for the control and prediction of the migration of pollutants in soils and groundwater. Information about speciation and adsorption of chemical species sorbed and in solution are needed to better understand the mechanisms.

The aim of this study was to investigate (poly)molybdate and (poly)tungstate ions sorption mechanism on various iron (hydr)oxide: hematite ( $\alpha\text{-Fe}_2\text{O}_3$ ), goethite ( $\alpha\text{-FeOOH}$ ), akaganeite ( $\beta\text{-FeOOH}$ ) and lepidocrocite ( $\gamma\text{-FeOOH}$ ). Attenuated Total Reflectance - infrared spectroscopy was used, which allowed *in situ* and real time analysis of surface adsorption [1,2]. Information about the surface reactivity of these various solids and the different behaviors of the ionic species have been investigated, and the influence of different experimental conditions (pH, concentration, ionic strength) were demonstrated. Our results show an important effect of the surface structure of the solids on the sorbed complex geometry : on lepidocrocite and goethite a monodentate structure is preferred, while a polymerization has been observed onto hematite surface. Both ions have a different behavior on akaganeite: molybdate ions polymerize while tungstate species seems to have the same monodentate structure than those found on goethite [3]. DFT study was used to confirmed the geometry of sorbed species with vibrational calculation.



**Figure 1:** In situ ATR-FTIR spectroscopy

- [1] Lefèvre (2004) *Adv. Colloid Interface Sci.* **107**, 109-123.  
 [2] Davantès & Lefèvre (2013) *J. Phys. Chem. A* **117**, 12922-12929. [3] Davantès & Lefèvre (accepted) *Eur. Phys. J. Special Topics*