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Surface speciation of the mono-molybdate/ lepidocrocite system by ATR-IR and polarized ATR-IR spectroscopy

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Oxoanion adsorption on metal oxides is an important phenomenon in several research domains, such as heterogeneous catalysis and geochemistry. Due to their polyatomic structure, they can be easily probed by mid infrared spectroscopy. For several years, we have developed an approach based on in situ and real time characterization of these species using Attenuated Total Reflectance - infrared spectroscopy. This technique allows us to record IR spectra of either dissolved or adsorbed species without any preparation of samples which could modify the surface speciation. The molybdate/lepidocrocite (g-FeOOH) system has been first studied using ATR-IR and DFT calculations of surface complexes [1]. In the present work, the surface speciation of molybdates has been refined, thanks to an extensive use of polarized ATR-IR [2].

This method requires a deposit of oriented particles, what is possible due to the lath-shaped geometry of lepidocrocite. The global anisotropy has been quantified using the experimental ratio of the transition dipolar moment of two FeOH bending modes, and compared with simulations by DFT calculations of lepidocrocite polarized spectra. Then, the differential spectra of molybdate species and surface hydroxyl groups as a function of pH and Mo concentration have been interpreted to give a full description of the adsorption mechanisms.

References:

[1] Davantès, Costa & Lefèvre (2016), *J. Phys. Chem. C* 120, 11871-11881.

[2] R. Botella & Lefèvre (2022), *Colloids Surfaces A.* 647, 129065.

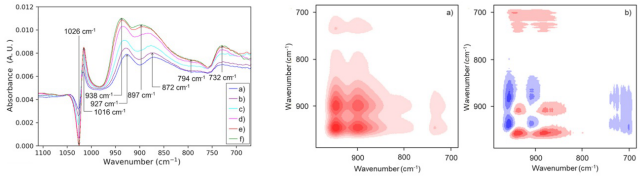

Fig. 1 Spectra for the lepidocrocite/molybdate 10^{-4} M system with decreasing pH from 6.0 to 3 (on the left) and (a) synchronous and (b) asynchronous 2D spectra for (on the right).