In-situ ATR-FTIR Kinetic Experiments and DFT Calculations on the Surface Chemistry of Oxyanions with Goethite and Hematite

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The surface chemistry of phosphorus and arsenic compounds in their organic and inorganic forms is of great interest to the scientific and industrial communities due to its role in controlling their transport, bioaccessibility and speciation. **Our goal** is to investigate fundamental properties of surface interactions of these oxyanions with metal (oxyhydr)oxide surfaces relevant to the petroleum industry. This surface phenomena is of interest because organoarsenicals bind to surface sites through their inorganic moieties.

We utilized the **surface-sensitive technique attenuated total internal reflectance Fourier transform infrared spectroscopy (ATR-FTIR)**. Spectroscopic signature of adsorbed DMA, arsenate and phosphate were analyzed for the kinetics of adsorption and desorption. Quantum mechanical calculations of the thermodynamics of binding using DFT/B3LYP method were also performed on cluster models to aid in the interpretation of experimental data.

Results show that pseudo adsorption rate constants increase in this order: arsenate-covered < DMA-covered ≤ freshly-prepared. Also, pseudo desorption rate constants of DMA complexes are 7-12 times higher than arsenate using phosphate as a desorbing agent.

Next, we will quantify the binding strength and kinetics of DMA to surface covered with organic acids.