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

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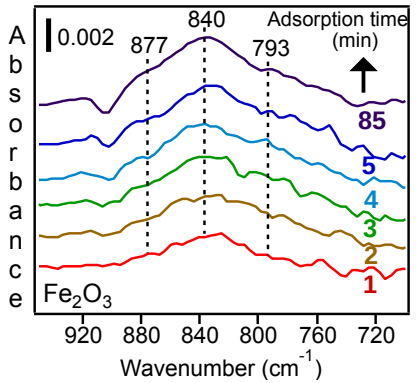
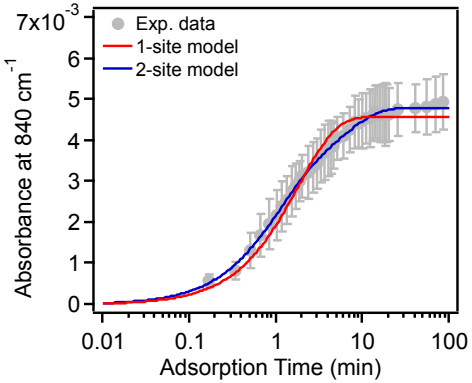
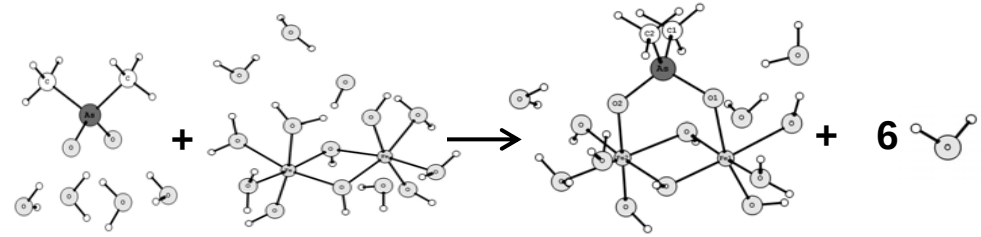
Dimethylarsinic Acid (DMA) belongs to an important class of methylated organoarsenical compounds that exist in fossil fuels and biomass as impurities of biogeochemical origins. They lower the purity of fuel and poison catalysts used in refinery processes. **Our goal** is to investigate fundamental properties of DMA interaction with metal (oxyhydr)oxide surfaces relevant to the petroleum industry.

We utilized the **surface-sensitive technique attenuated total internal reflectance Fourier transform infrared spectroscopy (ATR-FTIR)** to investigate the kinetics of DMA interaction with goethite and hematite particles. We also calculated the thermodynamics of binding using DFT/B3LYP method.







ΔG_{ads} = -145 kJ/mol

Example DFT/B3LYP calculations on the formation of the thermodynamically most stable DMA complex with iron clusters

Results show fast and slow adsorption rates from spectral data, consistent with the formation of more than one type of adsorbed DMA . Calculated values of ΔG_{des} indicate that desorption favorability of DMA complexes increases in this order: bidentate < mondentate < outersphere. **Next**, we will quantify the binding strength and kinetics of DMA to surface covered with organic acids.