

## **Molecular behavior of Cr(VI) on the Surface of Iron Phosphate mineral**

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A research was conducted to investigate the behavior of Cr(VI) on the surface of a ferrous phosphate (vivianite) in the molecular level. At neutral pH, a fast Cr(VI) removal kinetics was observed on the vivianite surface with the surface normalized rate constant (2.5–4.2 L m d ) higher than those of other Fe(II)containing minerals. The rate constant (35.37 ± 5.27 h ) at pH 5 was highest, which was 33 and 393 times higher than those at pH 7 and 9, indicating the enhanced reaction kinetics by the decrease of pH. The results obtained from X-ray spectroscopic results clearly verified that the continuous reduction of Cr(VI) on the vivianite surface with coupled oxidation of Fe(II) during the reaction. A theoretical estimation for the optimized structure of Cr(VI)-vivianite complexation by density functional theory was in good agreement with the structure obtained by extended X-ray absorption fine structure showing the transformation of vivianite to amorphous Fe(III) phosphate and favored Fe-A site for both Cr(VI) species (i.e., HCrO and CrO ) compared to Fe-B site on the surface of vivianite.