Investigation of Chromate Coordination Modes and Its Transformation Behaviors on Schwertmannite interface under environmental disturbance

ZHI DANG*, XIAOFEI LI, CHULING GUO

School of Environment and Energy, South China University of Technology, Guangzhou 510006, China

(*correspondence:chzdang@scut.edu.cn)

Chromate mobility and bioavailability in subsurface environment is strongly affected by interfacial reactions on iron-based minerals. Elucidation of the chromate surface complexation characteristics and its coordination configuration transformation under environmental disturbance will help to better understand its geochemical behavior in natural environment. In this study, batch adsorption/desorption experiments in combination with *in situ* attenuated total reflectance fourier transform infrared spectroscopy (ATR-FTIR), were employed to investigate the interaction mechanisms of chromate on water-schwertmannite (Sch) interface, whilst the multivariate curve resolution analysis (MCR) were used to enhance the resolution of ATR-FTIR bands and the accuracy of analysis. Results showed that the chromate adsorption capacity were non-continuous reduction with the increase of pH, and the maximum values appeared at pH range of 5.0-6.0 in batch adsorption experiments. The frequent desorption experiments displayed an obvious lower releasing percentage of chromate from adsorbed Sch at high pH, indicating a relative stable surface complexes formed. *In situ* ATR-FTIR spectroscopic results showed that the dominant adsorbed species of chromate was bidentate inner-sphere complexes (C_{2v}) in low pH, and its proportion reduced with increasing pH from 5.0 to 8.0, while the monodentate complexes (C_{3v}) gradually became the dominant configuration instead of outer-sphere complexes. In addition, chromate surface coverage exerted little influence on the surface complexes. The distribution of chromate complexes species and its transformation behaviors is important for predicting the fate and transport of dissolved chromate in AMD contaminated environments.