

Facet-dependent surface charge and Pb^{2+} adsorption characteristics of hematite: CD-MUSIC modeling

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Predicting the environmental fate of lead (Pb) relies on a detailed understanding of its coordination to mineral surfaces, which in turn reflects the innate reactivity of the mineral surface. In this research, we investigated the proton and Pb^{2+} adsorption and speciation of hematite nanoplates (HNP) and nanocubes (HNC) exposing the (012), (001), and/or (110) crystallographic facets. The electron microscope analysis revealed HNP was of ca. 85.5% (001) and 14.5% (012) facets, while HNC was of ca. 76.0% (012) and 24.0% (110) facets. CD-MUSIC model could describe both the proton and Pb^{2+} adsorption well with optimized parameters. The (012) and (110) facets exhibit larger proton charge density and Pb^{2+} adsorption capacity than the (001) facets. The detailed speciation of Pb on different hematite facets was explored by CD-MUSIC modeling.

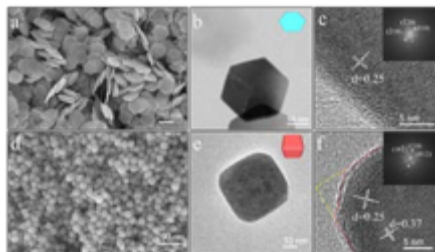


Fig. 1 Field emission scanning electron microscope (SEM) images of HNP (a) and HNC (d); high-resolution transmission electron microscopy (HRTEM) images of HNP (b, c) and HNC (e, f).

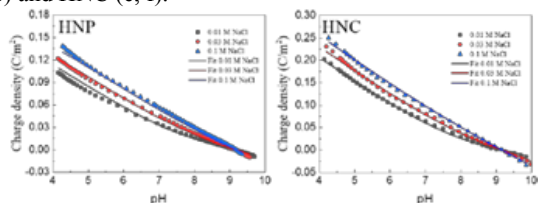


Fig. 2 Charge density (C/m^2) of HNP and HNC as a function of pH. The scatters represent data derived from the potentiometric titration experiments; the lines represent the CD-MUSIC model calculations.