

Interfacial phenomena of Al-substituted ferrihydrite

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Ferrihydrite is one of the most common iron oxy(hydr)oxides in the environment, occurring naturally in soils and sediments and as a result of acid mine drainage [1]. Due to its small particle size and unique surface characteristics, high surface area and site density, ferrihydrite is one of the most reactive nanominerals, regulating the mobility of the contaminants in aqueous environments [2]. Impurities in the bulk structure of ferrihydrite are quite ubiquitous in nature with aluminum to be one of the most common substituent for ferrihydrite [3]. The objective of this work is to investigate the implications of isomorphic substitution of Al to the ferrihydrite surface reactivity. A surface complexation model (SCM) is developed incorporating insights from mineral structure [3], spectroscopy [4] with a link to macroscopic observations.

Bompoti, et al. [5] developed an 3-site SCM to simulate proton reactivity of ferrihydrite nanoparticles using the CD-MUSIC framework [6]. This work integrates previous findings for ferrihydrite surface structure and pure aluminum oxide phases to construct a SCM for Al-ferrihydrite. The SCM is calibrated on surface charge curves and oxyanion adsorption data collected for 6, 12 and 18 mol% Al substitution. Hexavalent chromium (CrO_4^{2-}) was used as a model contaminant to quantify adsorption under pH conditions. Surface charge density curves showed a shift on Point of Zero Charge (PZC) while adsorption data indicated a lower reactivity in different Al contents. This work provides a discussion on the surface structure of the Al-ferrihydrite including SCM of surface charge and specific ion adsorption.

[1] Hiemstra and Van Riemsdijk (2009), *Geochimica et Cosmochimica Acta* 73, 4423–4436. [2] Davis et al. (1978), *Journal of Colloid and Interface Science* 63, 480–499. [3] Cismasu et al. (2012), *Geochimica et Cosmochimica Acta* 92, 275–291. [4] Johnston and Chrysochoou (2016), *Environ. Sci. Technol.* 50, 3589–3596. [5] Bompoti et al. (2017) *Chemical Geology* 464, 34–45. [6] Hiemstra and Van Riemsdijk (1996), *Journal of Colloid and Interface Science* 179, 488–508.