

Investigation of Surface Structures by Powder Diffraction: A Differential Pair Distribution Function (PDF) Study into Arsenate Sorption on Ferrihydrite

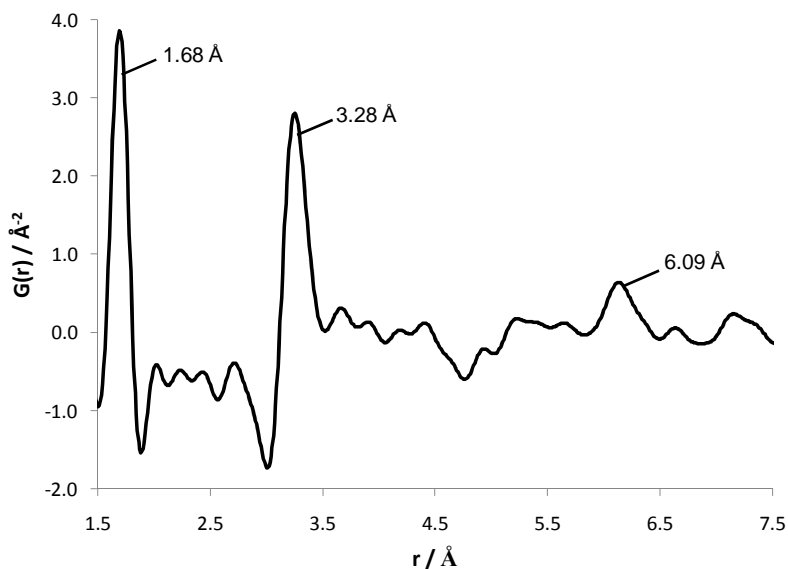
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We present a study into the structure of surface species on nanoparticles using differential Pair Distribution Function analysis of total x-ray scattering data.¹ In a typical powder diffraction experiment for PDF analysis a ‘blank’ diffraction pattern, consisting of the empty sample container is subtracted from the pattern of the sample, leaving only the scattering from the powder to be analysed. In this way, the parasitic scattering from the container and air scattering from the hutch, dismissed as background in Rietveld refinements, is removed from the data prior to analysis. In a differential PDF experiment, the blank is powder of a ‘host’ material which is subtracted from a pattern of a ‘host + guest’ sample, leaving guest-guest and guest-host interactions.

The system investigated in this report is arsenic(V) oxyanions (AsO_4^{3-}) sorbed on the surface of ferrihydrite, a naturally occurring iron oxyhydroxide nanoparticle. We observe features in the PDF confirming the bidentate binuclear attachment proposed by analysis EXAFS data.² We also observe a correlation at longer distances, arising due to an As-As distance on the surface of the particle (Figure).



¹Chapman, K. W., Chupas, P. J., Maxey, E. R. & Richardson, J. W. (2006). ChemComm 4013-4015.

²Sherman, D. M. & Randall, S. R. (2003). Geochimica et Cosmochimica Acta **67**, 4223-4230.