

# Supplementary Materials: The Binding of Phosphorus Species at Goethite: A Joint Experimental and Theoretical Study

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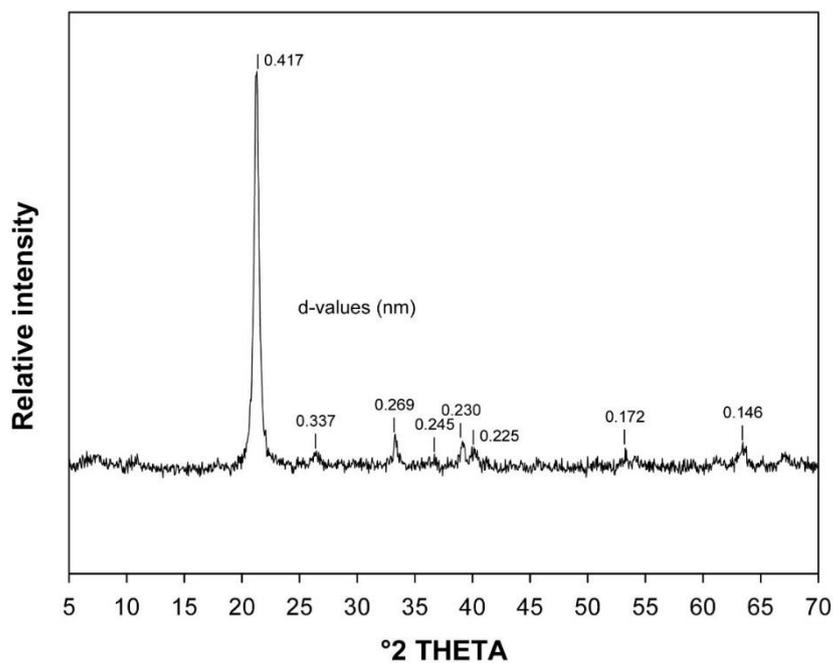


Figure S1. XRD pattern for pure goethite sample.

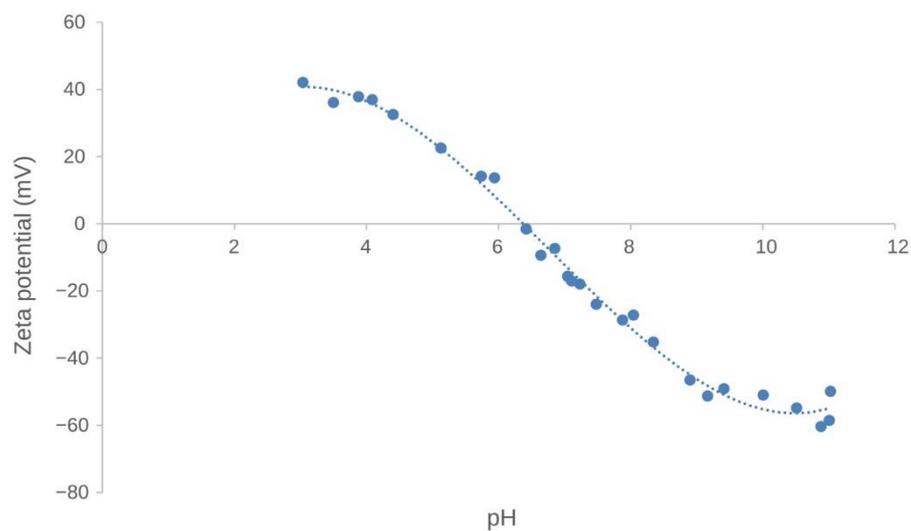
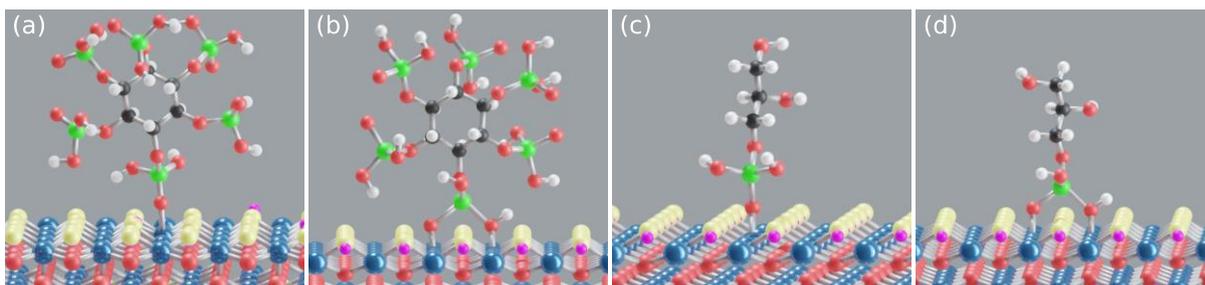
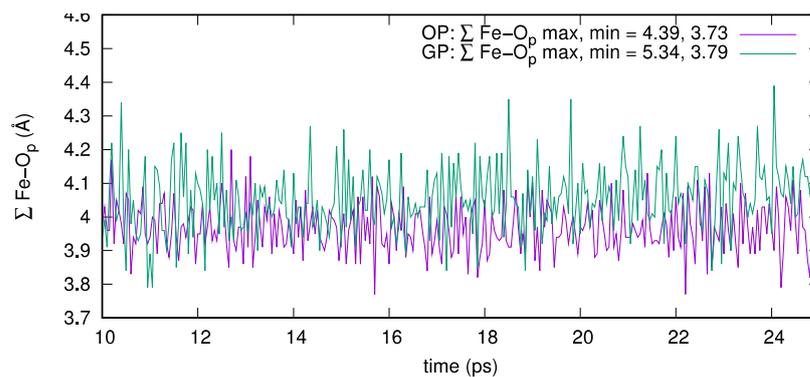


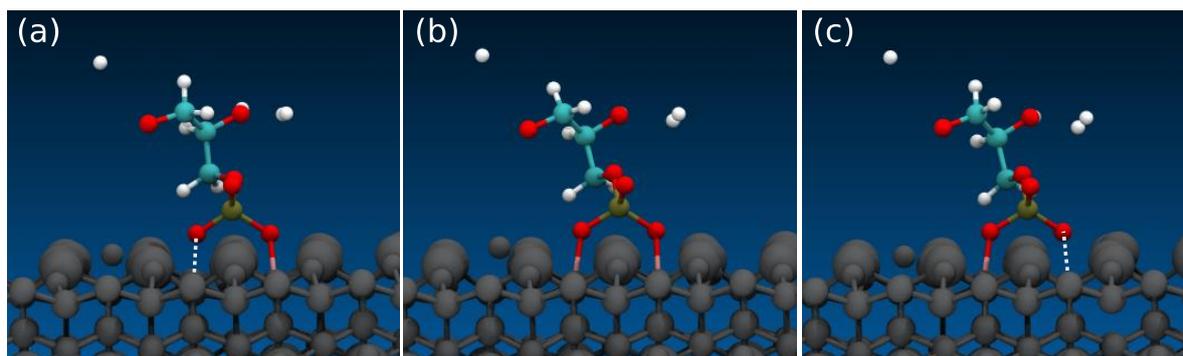
Figure S2. Effect of pH on electrophoretic zeta potential of goethite particles. Dashed line shows polynomial fitting to all data points representing the PZC of 6.3 ( $R^2 = 0.99$ ).



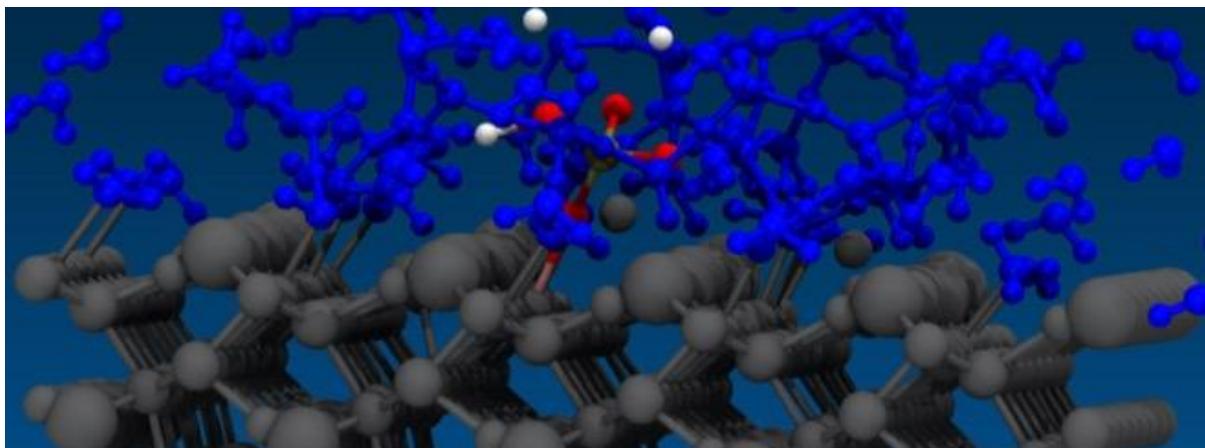
**Figure S3.** Initial motifs of IHP: **M**, **B** motifs (a,b) and GP **M**, **B** motifs (c,d).



**Figure S4.** Sum of Fe-O<sub>p</sub> bond lengths observed in goethite-OP and goethite-GP **B** motifs.



**Figure S5.** Seesaw movement of the bound GP's phosphate group to the goethite surface for the **B** motif case. (a) and (c) show momentarily elongated Fe-O bonds (left and right bonds, respectively) passing through a more stable **B** motif as shown in (b).



**Figure S6.** Multiple Fe-O<sub>water</sub> **M** motifs between water oxygens and surface Fe atoms on goethite.