Supplementary Information:
Ab Initio Molecular Dynamics Simulations of the Interaction between Organic Phosphates and Goethite

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FIGURES

Figure S1: Fitted IR spectra of IHP bonded through M (a) and 3M motifs (b).
Figure S2: Comparison of GP and IHP spectra with experimental spectra from Li et al. [29] and Yan et al. [41] studies, respectively. The blue rectangle denotes region within ±15 cm$^{-1}$ around frequencies observed in experimental studies.

Figure S3: Initial motifs of IHP: M motif (a), B motif (b).
Figure S4: GP BB motif (a), HBs (yellow dotted lines) between GP and surrounding water (b), water bonded to surface Fe atoms (c). Pink, red, yellow, white and lime colors correspond to iron, oxygen, hydroxyl oxygen, hydrogen and phosphorus, respectively.

Figure S5: Pair correlation function calculated for surface Fe atoms of goethite and oxygens of water observed for GP M motif case.
Figure S6: Covalent bond lengths of Fe-O \( P \) bonds for GP \( M(\text{Fe–O}_P) \) and B(Fe–O\(_{P1}\), Fe–O\(_{P2}\)) motifs (a,b) and IHP \( M(\text{Fe–O}_P) \) and \( 3M(\text{Fe–O}_P, \text{Fe–O}_{P1}, \text{Fe–O}_{P2}, \text{Fe–O}_{P3}) \) motifs (c,d) between 25–55 ps.

Figure S7: Binding energies along the simulation trajectory of IHP \( M \) motif in the time range of 25–50 ps.