Iron in Hydroxyapatite: Interstitial or Substitution Sites?

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SUPPLEMENTARY INFORMATION

Table S1. Chemical potentials in eV at selected points from the phase stability diagram (Figure 2 of main text).

P_i	$\mu_{\mathrm{Ca}}-\mu^0_{\mathrm{Ca}}$	$\mu_{\mathrm{P}}-\mu^0_{\mathrm{P}}$	$\mu_{\mathrm{O}}-\mu^0_{\mathrm{O}}$	$\mu_{\mathrm{H}}-\mu^0_{\mathrm{H}}$	**Coexisting phases**
P_1	−6.0	−10.8	0.0	−1.8	O_2, $Ca(OH)_2$, CaO
P_2	−6.0	−10.5	0.0	−2.6	O_2, CaO, TCP
P_3	−7.8	−7.9	0.0	−1.7	O_2, DCPA, TCP
P_4	−7.7	−8.1	0.0	−1.6	O_2, DCPA, DCPD
P_5	−6.7	−9.8	0.0	−1.5	O_2, $Ca(OH)_2$, DCPD
P_6	−2.4	−1.8	−3.6	0.0	H_2, $Ca(OH)_2$, CaO
P_7	−1.8	0.0	−4.3	0.0	H_2, CaO, P
P_8	−1.8	0.0	−4.2	−0.5	CaO, P, TCP
P_9	−4.7	0.0	−3.1	−0.2	DCPA, P, TCP
P_{10}	−4.5	0.0	−3.2	0.0	H_2, DCPA, DCPD, P
P_{11}	−3.7	−2.5	−2.9	0.0	H_2, $Ca(OH)_2$, DCPD

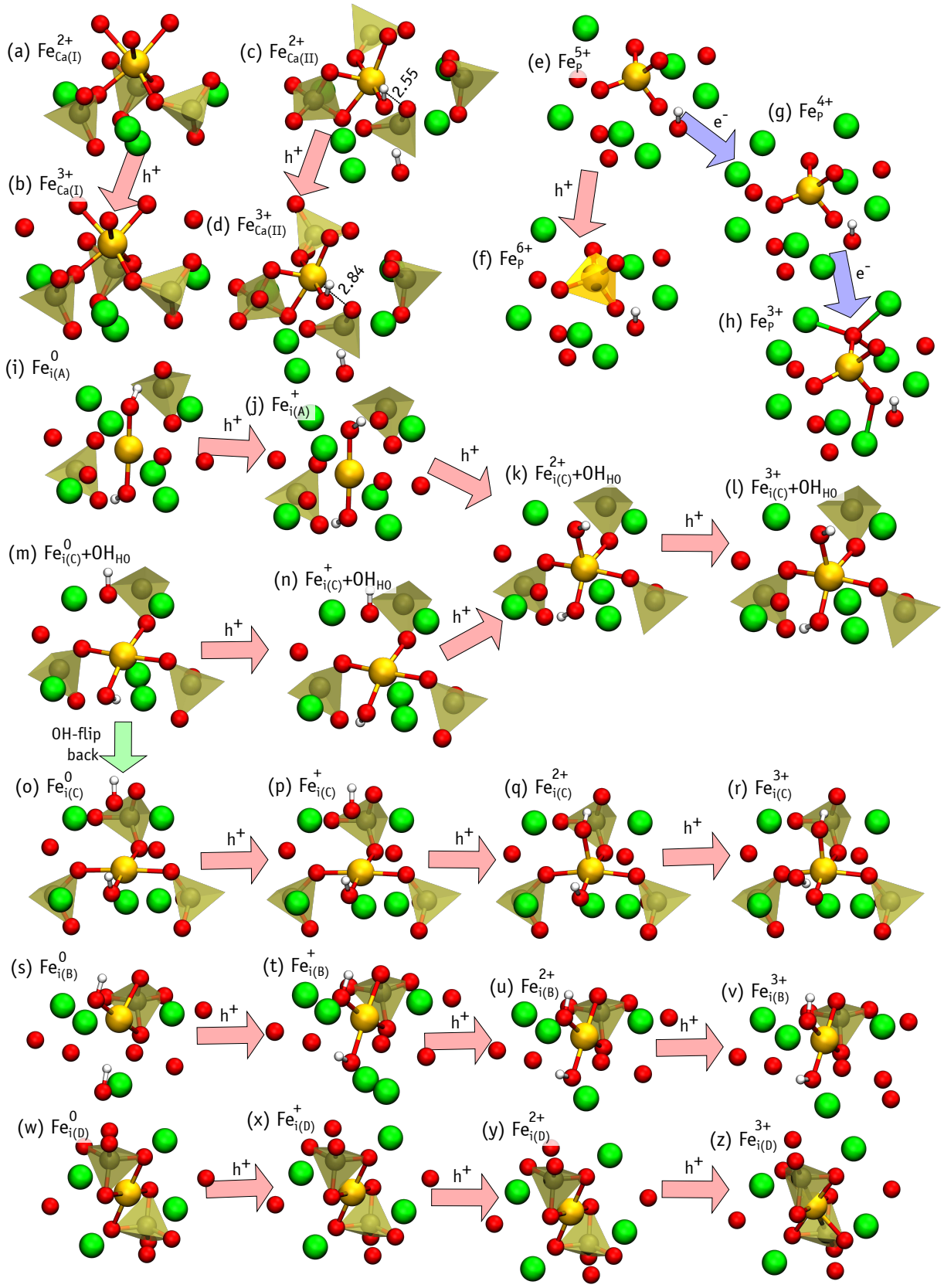

Figure S1. Illustration of the local atomic structure of iron atom ($\lesssim 4$ Å) for all considered Fe-HAp configurations. Iron, oxygen, calcium, hydrogen and phosphorus are shown in yellow, red, green, white, and inside the tetrahedra.

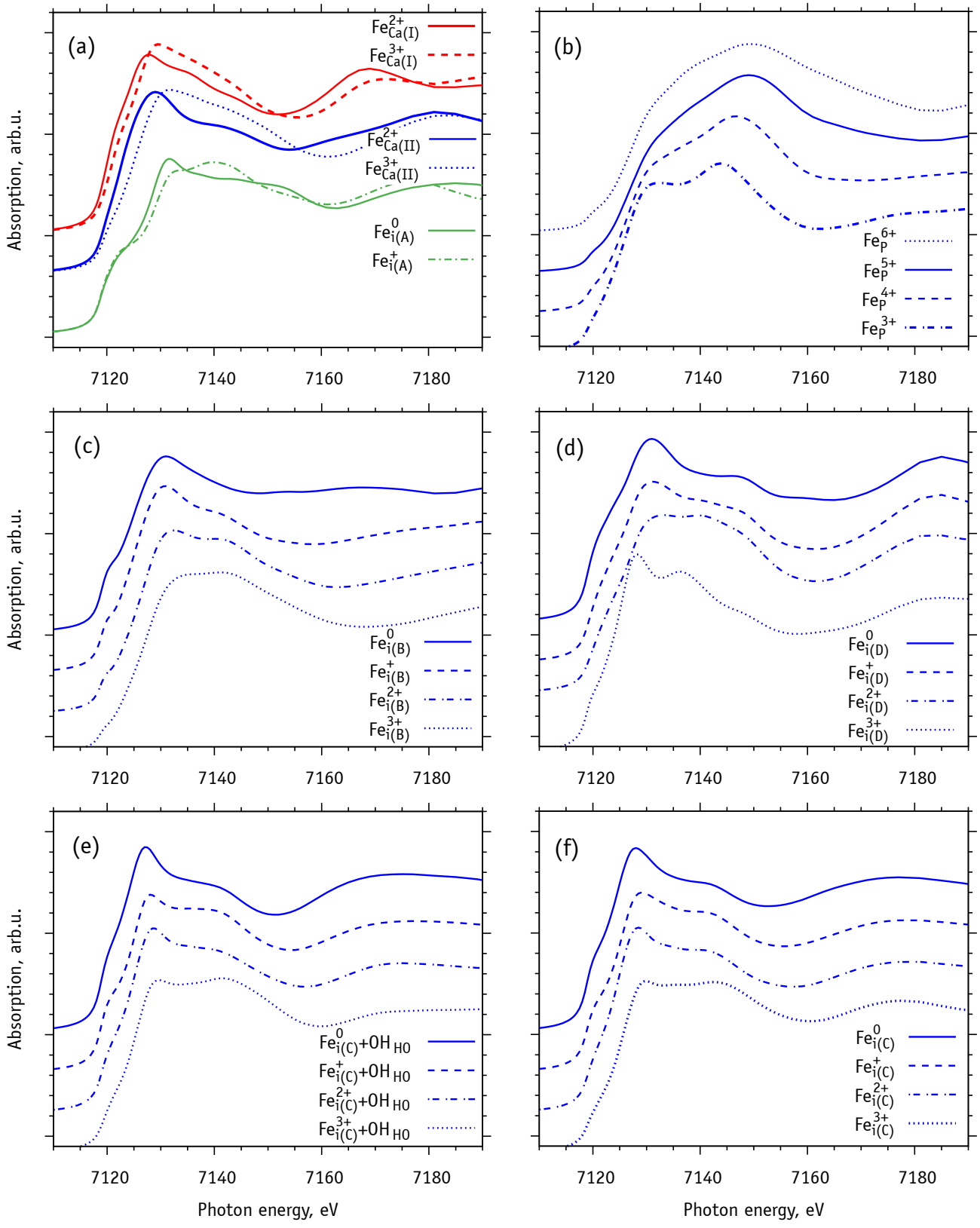

Figure S2. Simulated Fe K-XANES spectra for the considered Fe-HAp structures.