## An experimental–computer modeling study of inorganic phosphates surface adsorption on hydroxyapatite particles

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**Figure S1.** Morphology of particles synthesized for this study: (a) cHAp and (b) ACP. Left and right show low and high resolution SEM micrographs.



**Figure S2.** X-ray diffraction patterns of the HAp particles prepared in this work: ACP and cHAp. The hydroxyapatite was identified by the peaks at  $2\theta$  between 31.5° and 34.5°.



**Figure S3.** Proton-buffering capacity of the cHAp and ACP particles prepared in this work.



Figure S4. FTIR spectra of cHAp, ACP, polyP,  $P_2O_7^{4-}$  and ATMP.



**Figure S5.** High-resolution XPS spectra in the O1s region for cHAp samples before and after incubation in presence of polyP (200 mM; top),  $P_2O_7^{4-}$  (100 mM; middle) and ATMP (200 mM; bottom) at pH 7.



**Figure S6.** SEM micrographs of cHAp and ACP particles after incubation in presence of concentrated polyP (2 M),  $P_2O_7^{4-}$  (1 M) and ATMP (2 M; bottom) solutions at pH 7: (a) cHAp + polyP; (b) ACP + polyP; (c) cHAp +  $P_2O_7^{4-}$ ; (d) ACP +  $P_2O_7^{4-}$ ; (e) cHAp + ATMP; and (f) ACP + ATMP. Crystals of polyP,  $P_2O_7^{4-}$  and ATMP grown onto the surface of cHAp and ACP particles are indicated by arrows.