Adsorption of HPO_x and $CaHPO_x$ (x=1,. . . ,4) Molecules on Anatase TiO_2 (001) Surfaces

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Highlights

- $CaHPO_x$ and HPO_x adsorption on TiO_2 substrate is mostly ionic.
- HPO_x electronegativity increases with x and enhances electron transfer from the substrate.
- Electropositive, isolated Ca adatoms transfer electrons to Ti atoms of substrate bulk.
- Ca adatoms on TiO_2 favour HPO_4 adsorption and $CaHPO_4$ formation, and therefore osseointegration.