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Adsorption of HPO_x and CaHPO_x ($x=1, \dots, 4$) 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.

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