

Abstract Submitted  
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**Electronic Structure of Ti substituted hydroxyapatite: TiHap<sup>1</sup>**

SHUXIA YIN, DONALD ELLIS, Northwestern University — Hydroxyapatite (Hap), with the chemical formula  $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ , is the main mineral constituent of mammal tooth enamel and bone and has become an important biomaterial with medical applications. Hap also attracts increasing interest for use in environmental adsorbents and catalysts due to its porous nature and highly active ion-exchange character. Ti-modified Hap (TiHap) has been proved to possess high affinity to organic molecules and bacteria as well as high photocatalytic activity for their oxidative decomposition. The concentration of  $\text{Ti}^{4+}$  is a key factor controlling TiHap crystallinity and catalytic efficiency. Here we studied the sorption mechanism of  $\text{Ti}^{4+}$  on Hap using Density Functional Theory within periodic slab models.  $\text{Ti}^{4+}$  or  $(\text{Ti}(\text{OH})_2)^{2+}$ , as the most likely ion exchange species with  $\text{Ca}^{2+}$ , were first considered in bulk Hap. A second charge compensated model considered includes both surface Ca ion vacancies and substitutional  $\text{Ti}^{4+}$ . To obtain insight of the energetic stability and microscopic crystal structure of TiHap, Ti substitution on different Ca sites and distributions at different atomic ratios are investigated in both bulk and surface models.

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