Supplementary information

for

Probing the surface structure of hydroxyapatite through its interaction with hydroxyl: A first-principles study

Xian Wang, Li Zhang, Zeyu Liu, Qun Zeng, Gang Jiang and Mingli Yang*

Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China

* Corresponding author. Tel.: + 86-28-85405515; fax: + 86-28-85405515; E-mail address: myang@scu.edu.cn (Mingli Yang)

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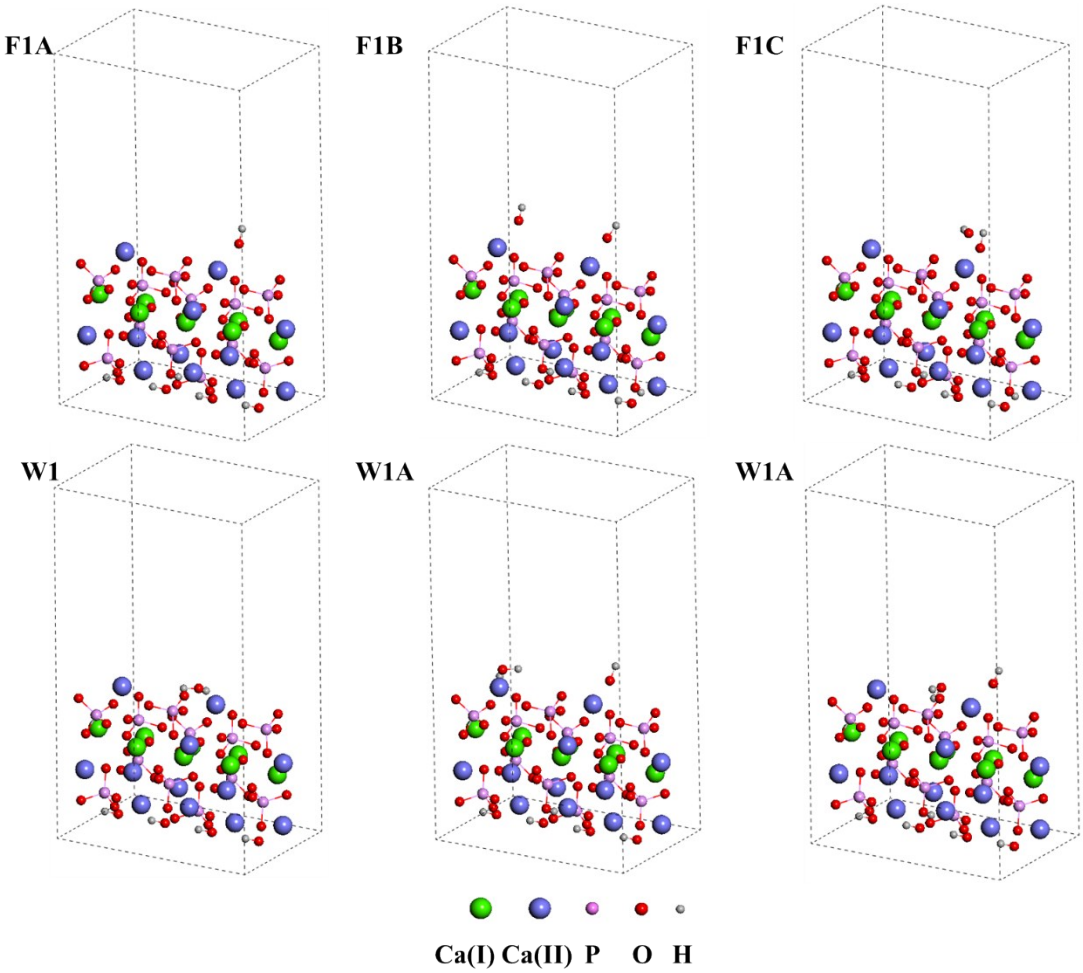

Fig. S1 Interaction patterns of hydroxyls (F1A, F1B and F1C), water molecule (W1), hydroxyl and water (W1A and W1B) on the Ca-rich (100) facet of HAp

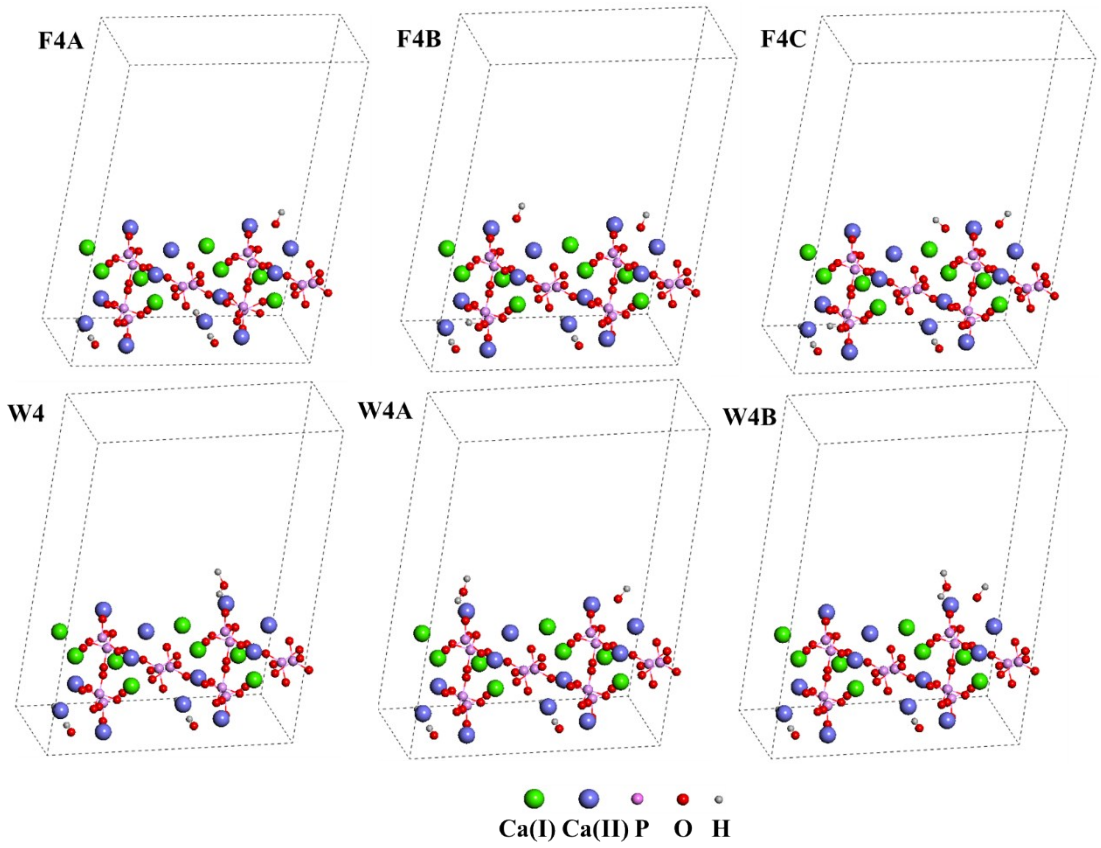

Fig. S2 Interaction patterns of hydroxyls (F4A, F4B and F4C), water molecule (W4), hydroxyl and water (W4A and W4B) on the Ca-rich (010) facet of HAp

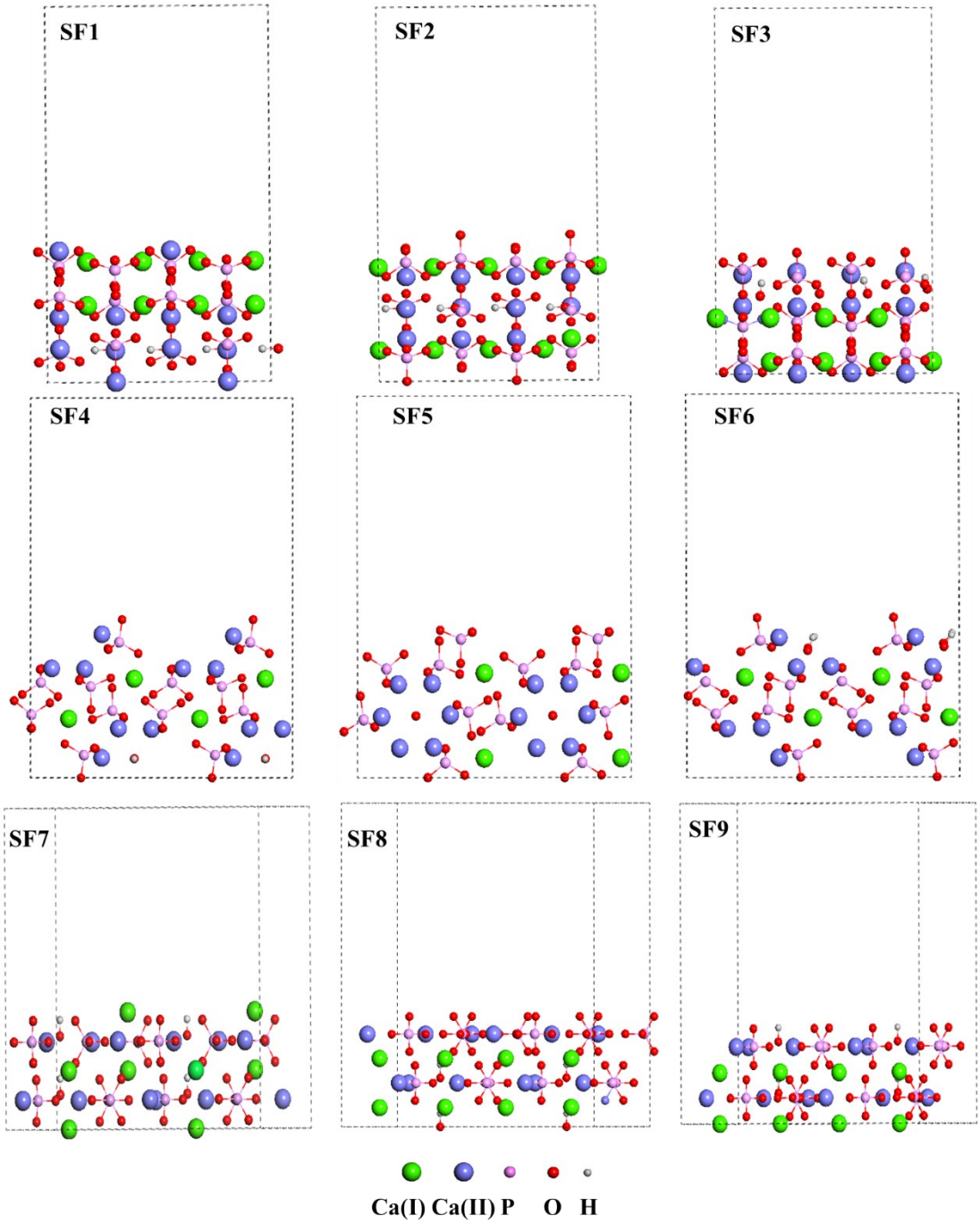

Fig. S3 Surface structures of pure HAp. SF1, SF2 and SF3 are Ca-rich, PO_4-rich and Ca-PO_4-OH surfaces on the (100) facet, respectively. SF4, SF5 and SF6 are Ca-rich, PO_4-rich and Ca-PO_4-OH surfaces on the (010) facet, respectively. SF7, SF8 and SF9 are Ca-rich, PO_4-rich and Ca-PO_4-OH surfaces on the (001) facet, respectively