Supporting information

First principles calculations on the hydrogen atom passivation of TiO2 nanotube

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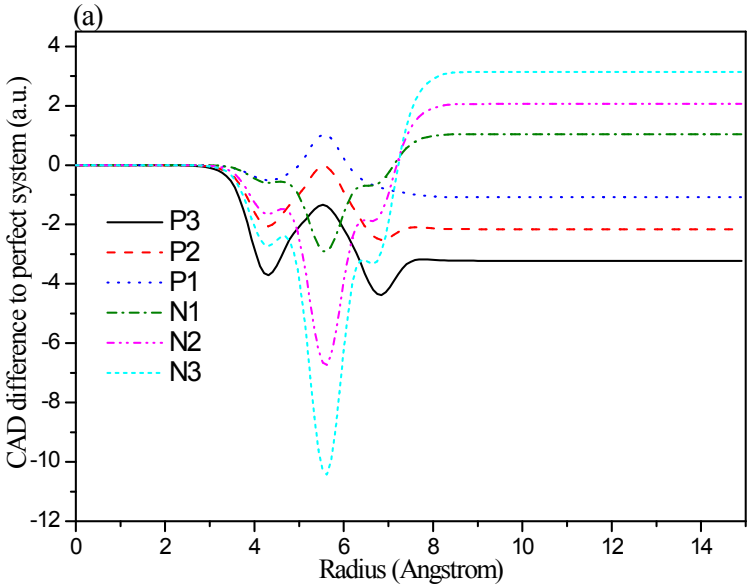
Fig. S1 The distributions of CAD difference of charged TiO_2 nanotubes. (a) (9, 0) and (b) (0, 6).



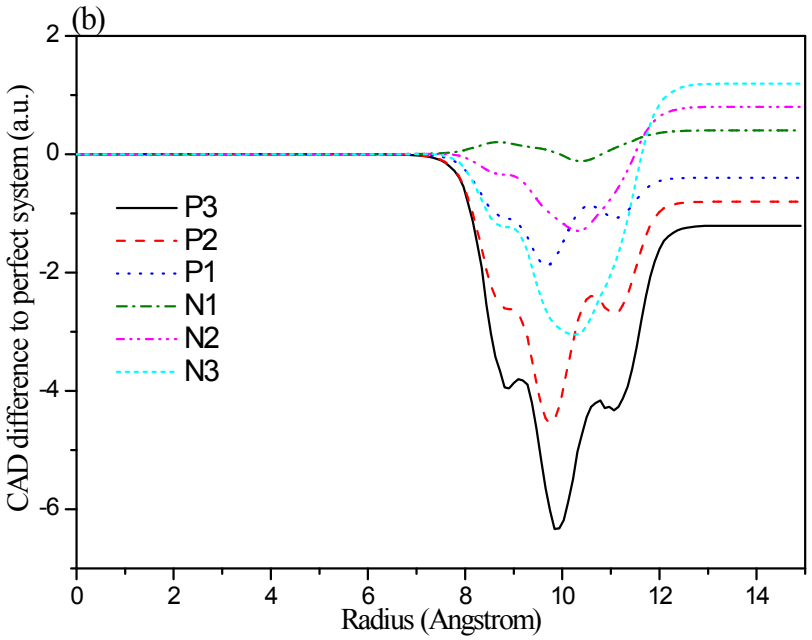


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Fig. S2 The charge difference distributions of charged TiO_2 nanotubes. (a) (9, 0) and (b) (0, 6).

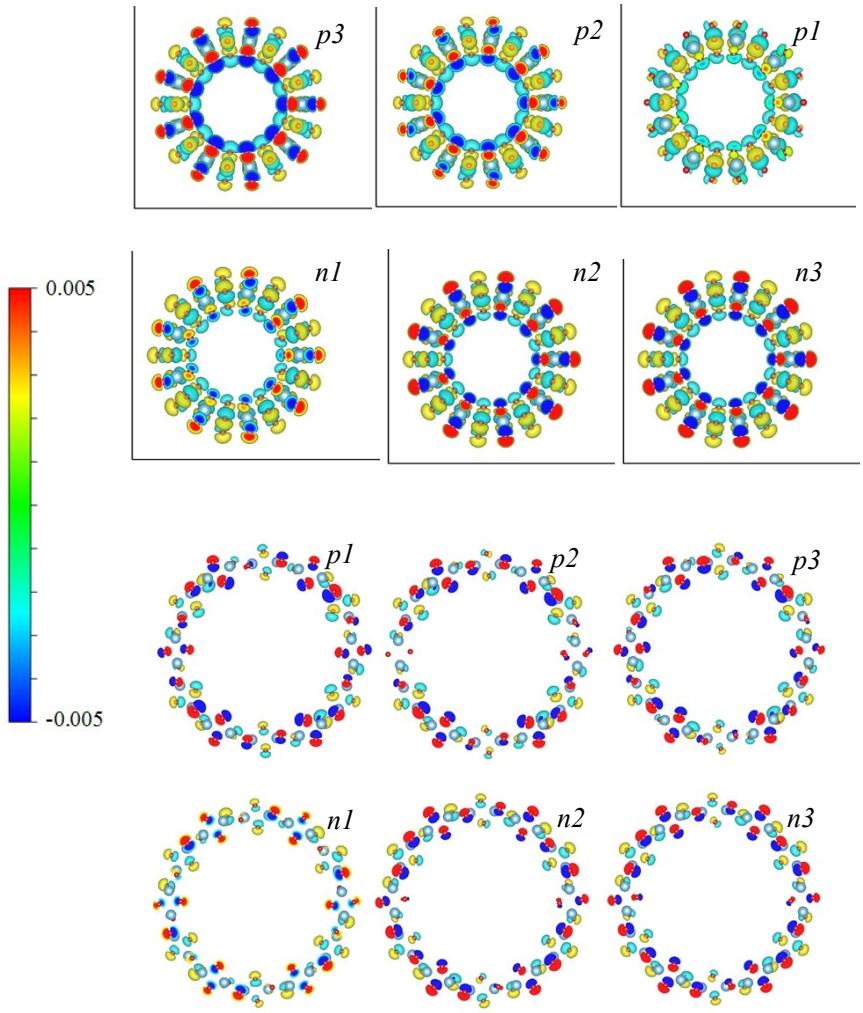

Fig. S3 The density of states of charged (9, 0) TiO_2 nanotube, (a) total density of states, (b) and (c) are the partial density of states of O and Ti atom in the (9, 0) TiO_2 nanotube, respectively.

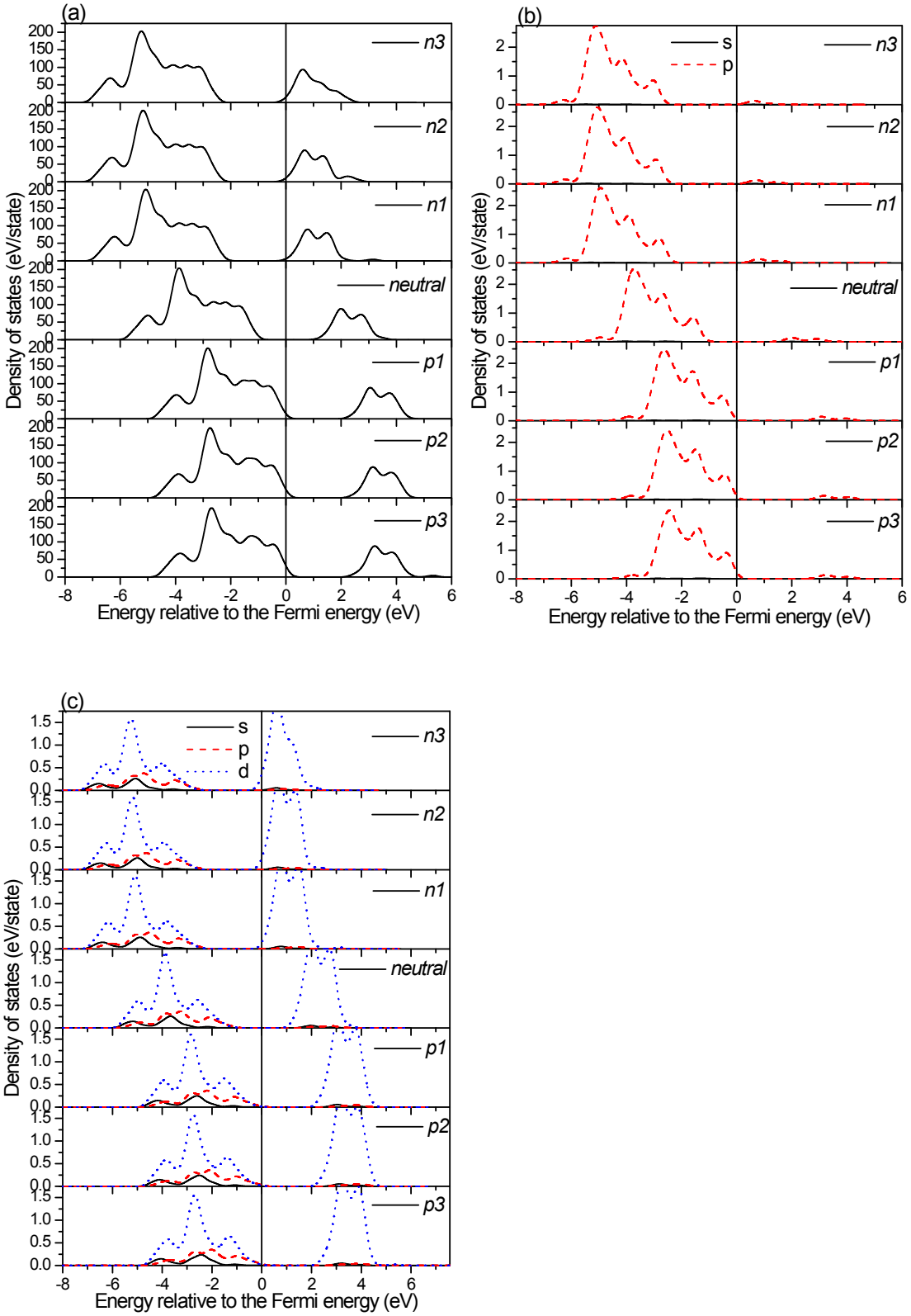

Fig. S4 The density of states of charged (0, 6) TiO_2 nanotube, (a) total density of states, (b) and (c) is the partial density of states of O, and Ti atom in the (0, 6) TiO_2 nanotube, respectively.

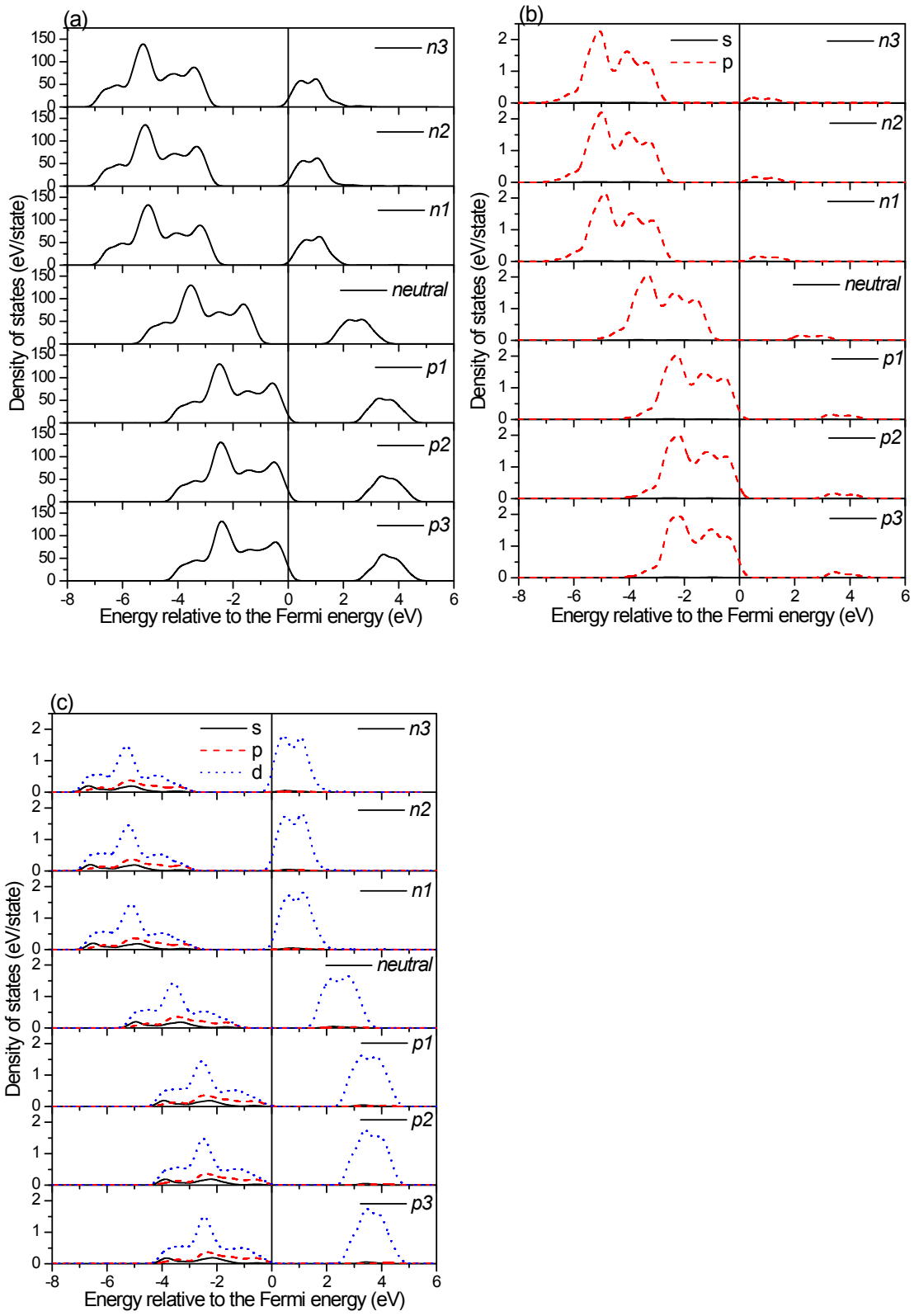

Fig. S5 The distributions of ELF of charged TiO_2 nanotubes.