Supporting Information

Insight into the effect of anionic–anionic co-doping on $BaTiO_3$ for visible light photocatalytic water splitting: A first principles hybrid computational study

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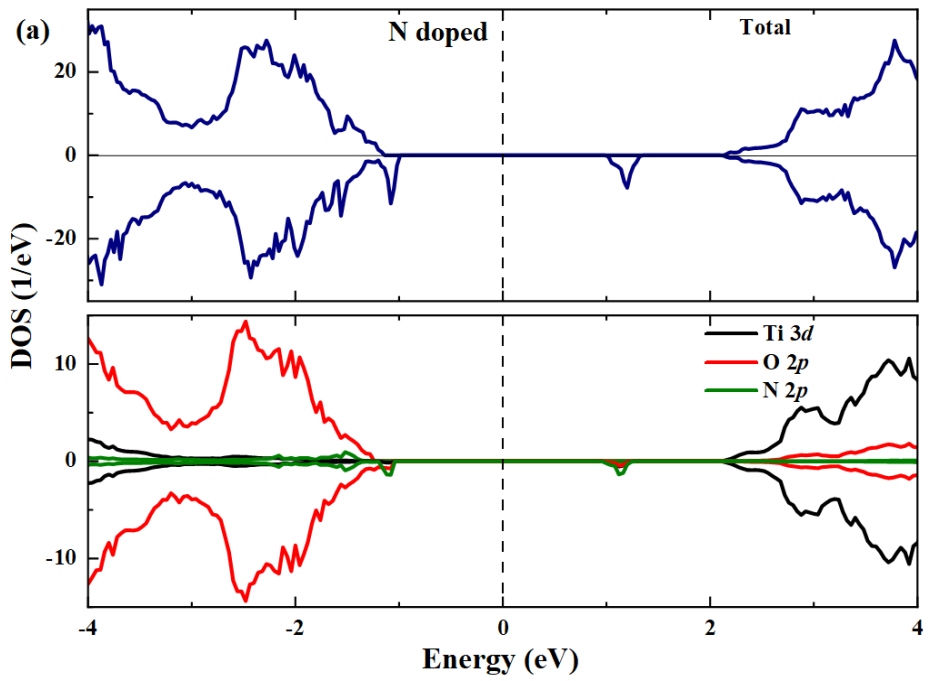
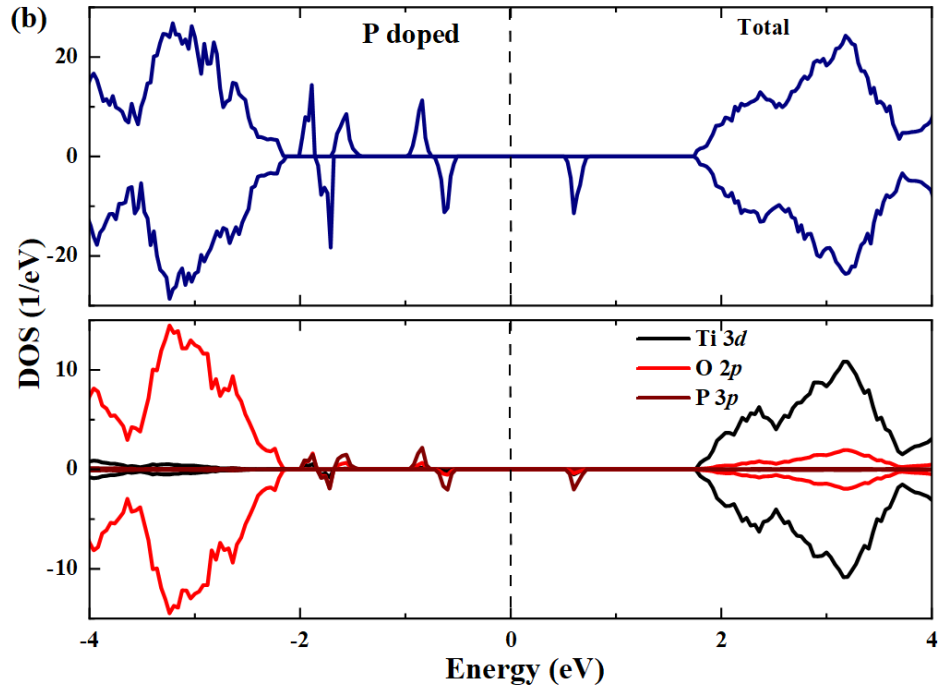

(a)
N doped
Total
DOS (1/eV)
Ti 3d
O 2p
N 2p
Energy (eV)


(b)
P doped
Total
DOS (1/eV)
Ti 3d
O 2p
P 3p
Energy (eV)

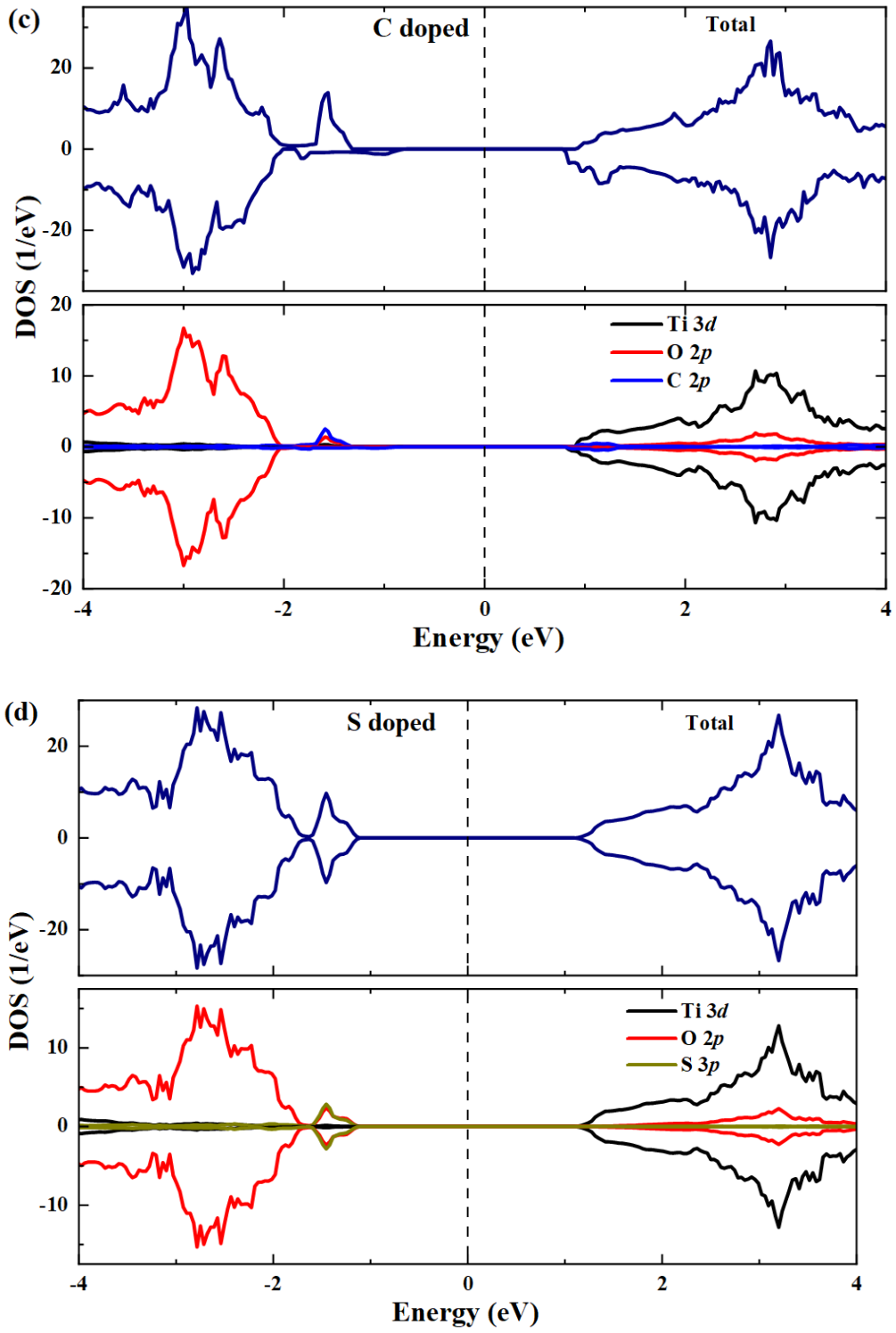


Figure S1. Calculated total and partial DOS of (a) N doped, (b) P doped, (c) C doped and (d) S doped $BaTiO_3$. Here, the vertical dashed line denotes the Fermi level

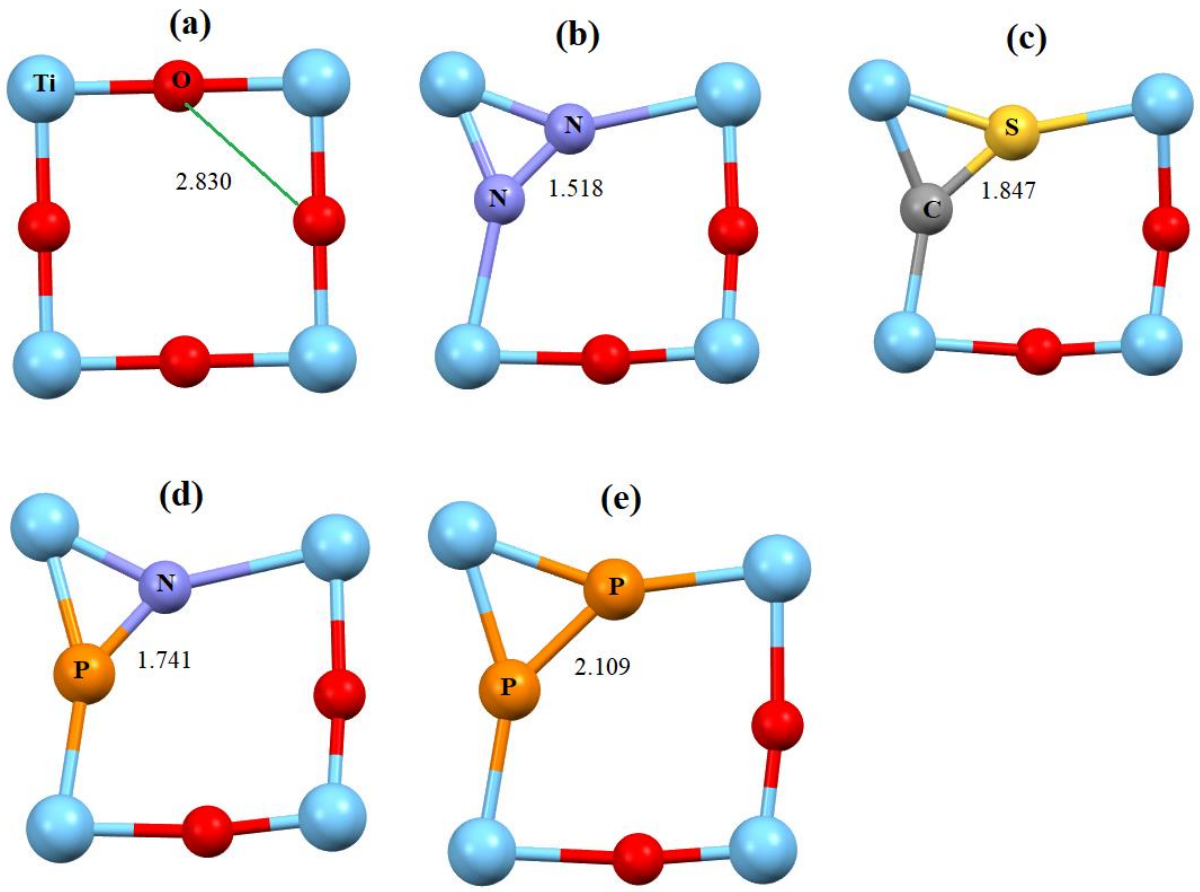


Figure S2. Side view of the optimized structures of (a) pristine, (b) N−N, (c) C−S, (d) N−P and (e) P−P co-doped $BaTiO_3$