

Supporting Information

Effect of metal decoration on sulfur-based gas molecules adsorption on phosphorene

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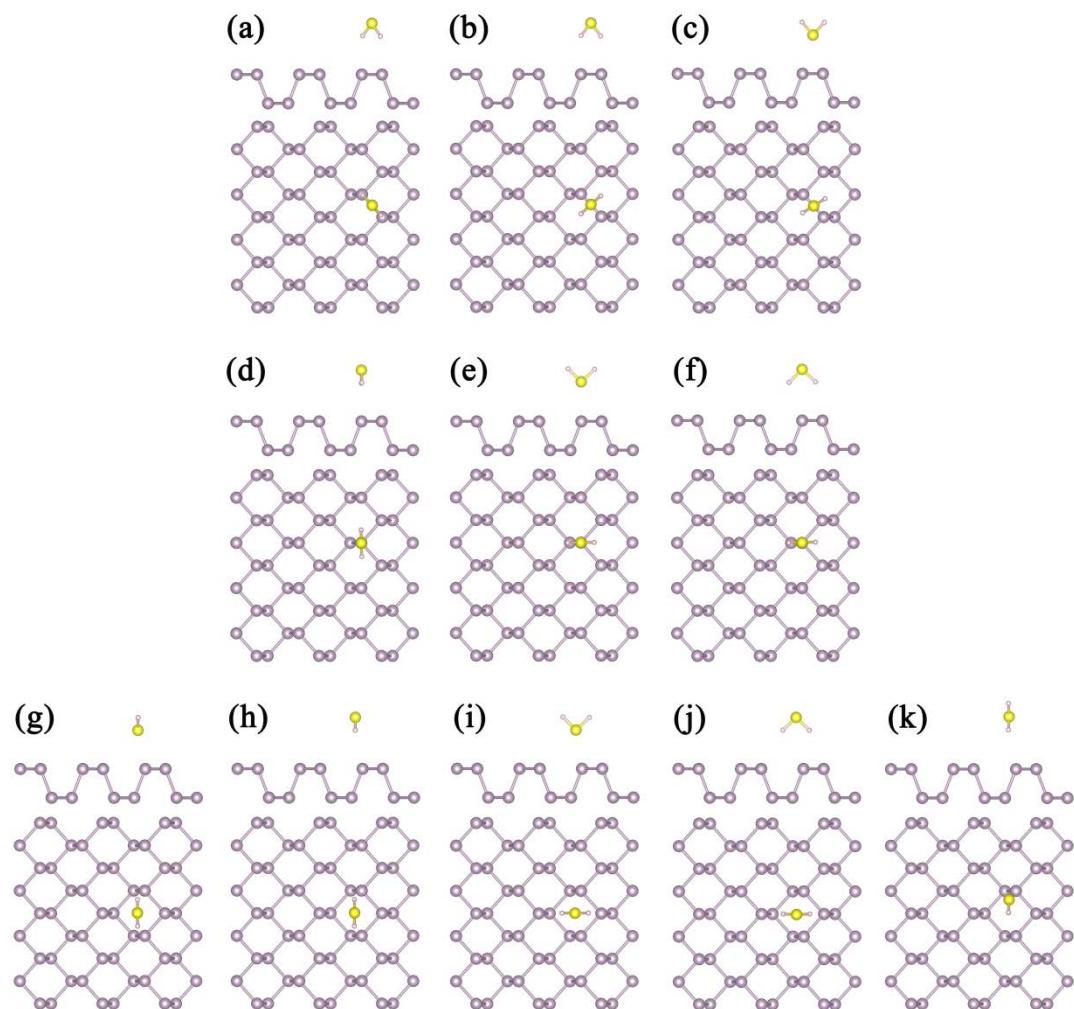


Figure S1. The initial structures of H_2S absorbed on 3×4 pristine phosphorene in different adsorption sites. (a)~(c) S atoms on bridge sites and H-H lines parallel to phosphorene plane with S atoms towards different directions; (d)~(f) S atoms on top sites and H-H lines parallel to phosphorene planes with S atom towards different directions; (g)~(j) S atoms on hollow sites and H-H lines parallel to phosphorene planes with S atom towards different directions; (k) H-H line vertical to phosphorene plane. Purple, yellow and white balls represent P, S and H atoms, respectively.

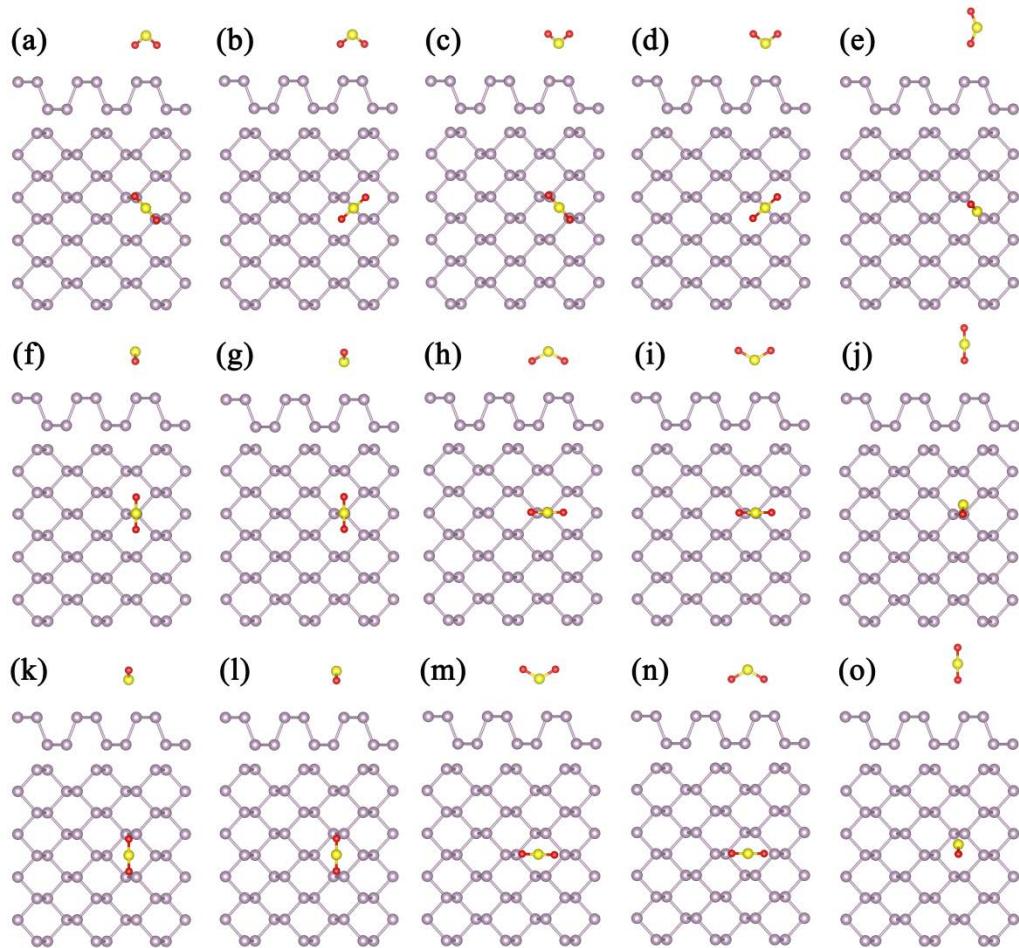


Figure S2. The initial structures of SO_2 adsorbed on 3×4 pristine phosphorene in different adsorption sites. (a)~(d) S atoms on bridge sites and O-O lines parallel to phosphorene planes with S towards different directions; (f)~(i) S atoms on top sites and O-O lines parallel to phosphorene planes with S towards different directions; (k)~(n) S atoms on hollow sites and O-O lines parallel to phosphorene planes with S towards different directions; O-O lines vertical to phosphorene planes with O atoms on (e) bridge, (j) top and (o) hollow sites. Purple, yellow and red balls represent P, S,

O atoms, respectively.

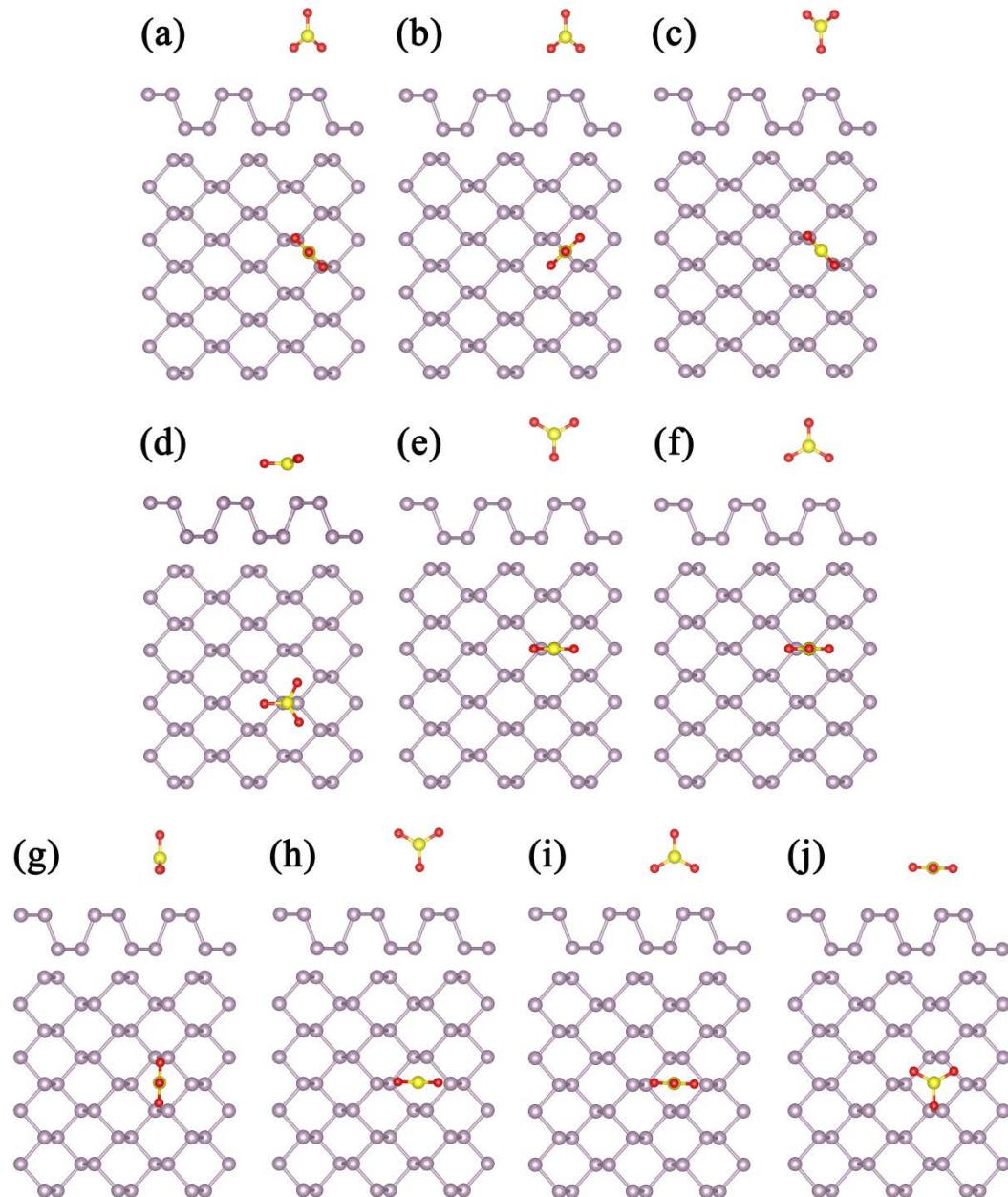


Figure S3. The initial structures of SO_3 absorbed on 3×4 pristine phosphorene in different adsorption sites. S atoms on bridge sites with O-S-O bond angle (a)-(b) toward phosphorene plane and (c) toward outside; S atoms on top sites with (d) O-atomic plane parallel to phosphorene plane, with O-S-O bond angle toward (e) outside and (f) phosphorene plane; S atoms on hollow sites with O-atomic planes (g)-(i) perpendicular and (j) parallel to phosphorene planes. Purple, yellow and red balls represent P, S, O atoms, respectively.

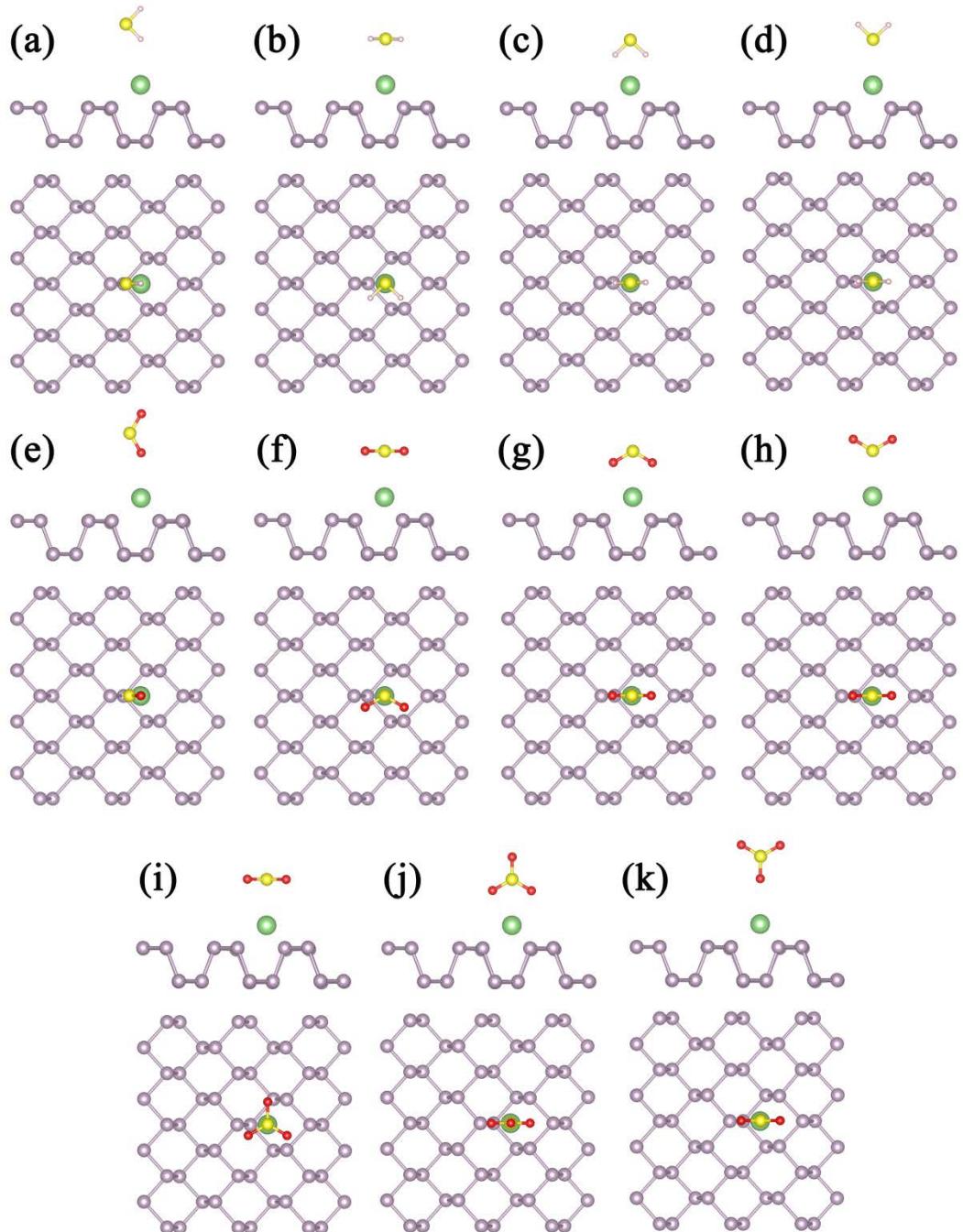


Figure S4. The initial structures of (a)-(d) H_2S , (e)-(h) SO_2 , (i)-(k) SO_3 absorbed on Li doped phosphorenes. Purple, yellow, white, red and green balls represent P, S, H, O and Li atoms, respectively.

Figure S5. The band structures of H₂S adsorption on bP-M (M=Li, Na, K, Rb, Cs, Ca, Sr, Ba, Ni, La, Tl). The red and blue curves represent the spin-up and spin-down bands, respectively. The Fermi level is set to zero.

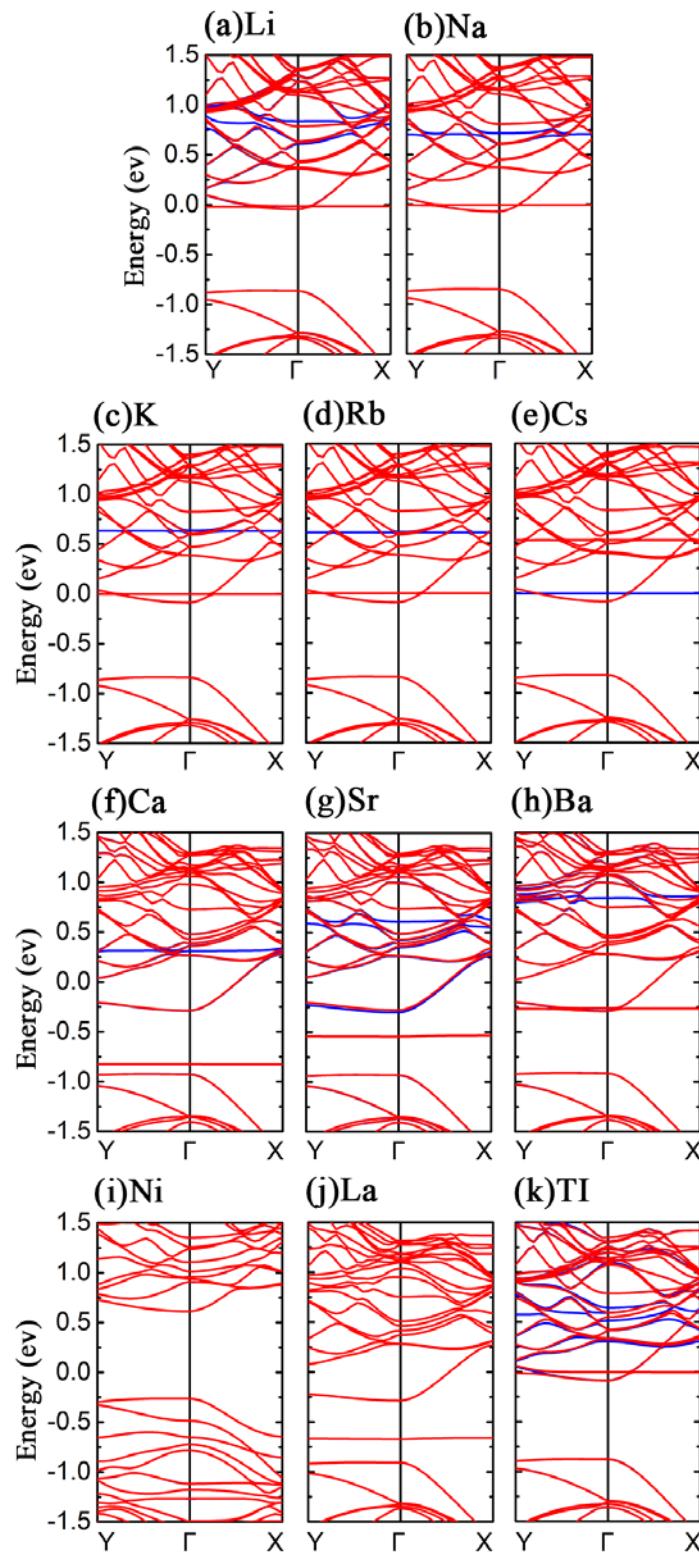


Figure S6. The band structures of SO_2 adsorption on bP-M (M=Li, Na, K, Rb, Cs, Ca, Sr, Ba, Ni, La, Tl). The red and blue curves represent the spin-up and spin-down bands, respectively. The Fermi level is set to zero.

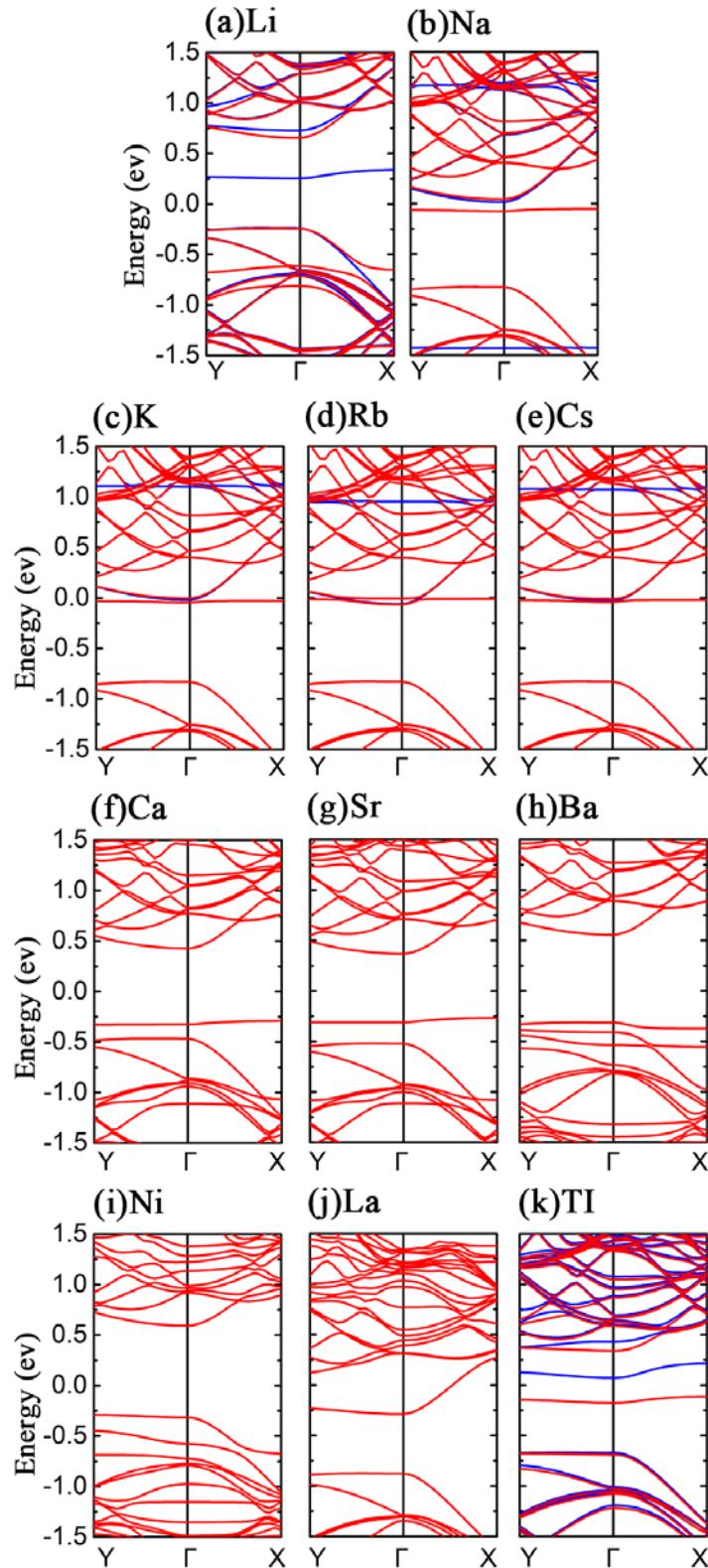


Figure S7. The band structures of SO_3 adsorption on bP-M (M=Li, Na, K, Rb, Cs, Ca, Sr, Ba, Ni, La, Ti). The red and blue curves represent the spin-up and spin-down bands, respectively. The Fermi level is set to zero.