

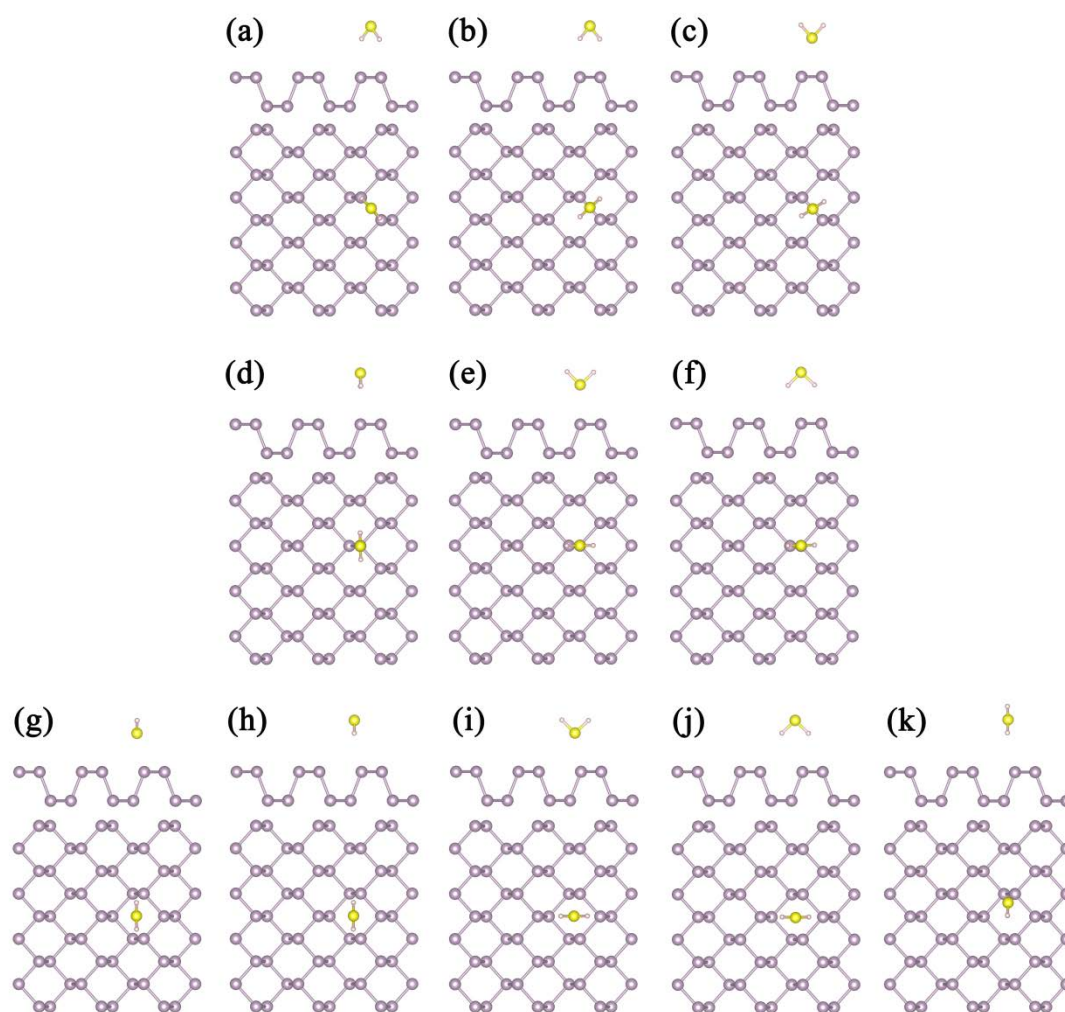
# Supporting Information

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

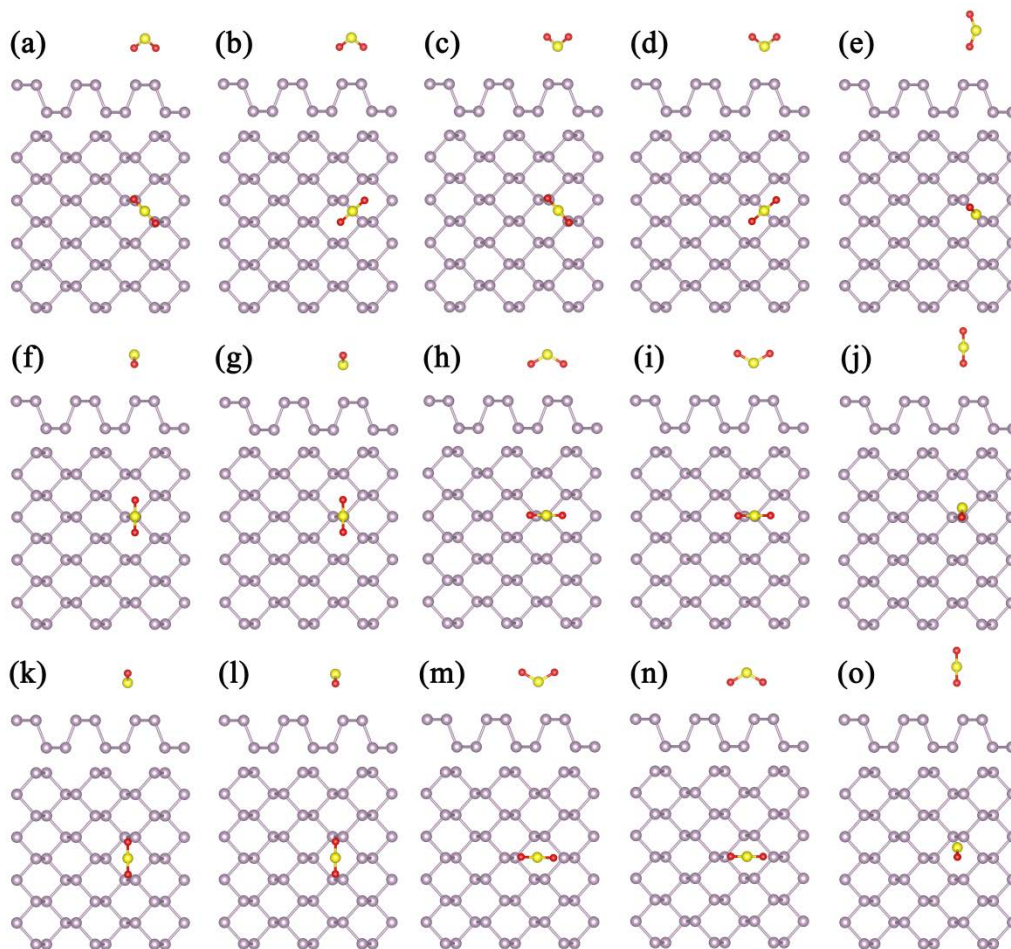
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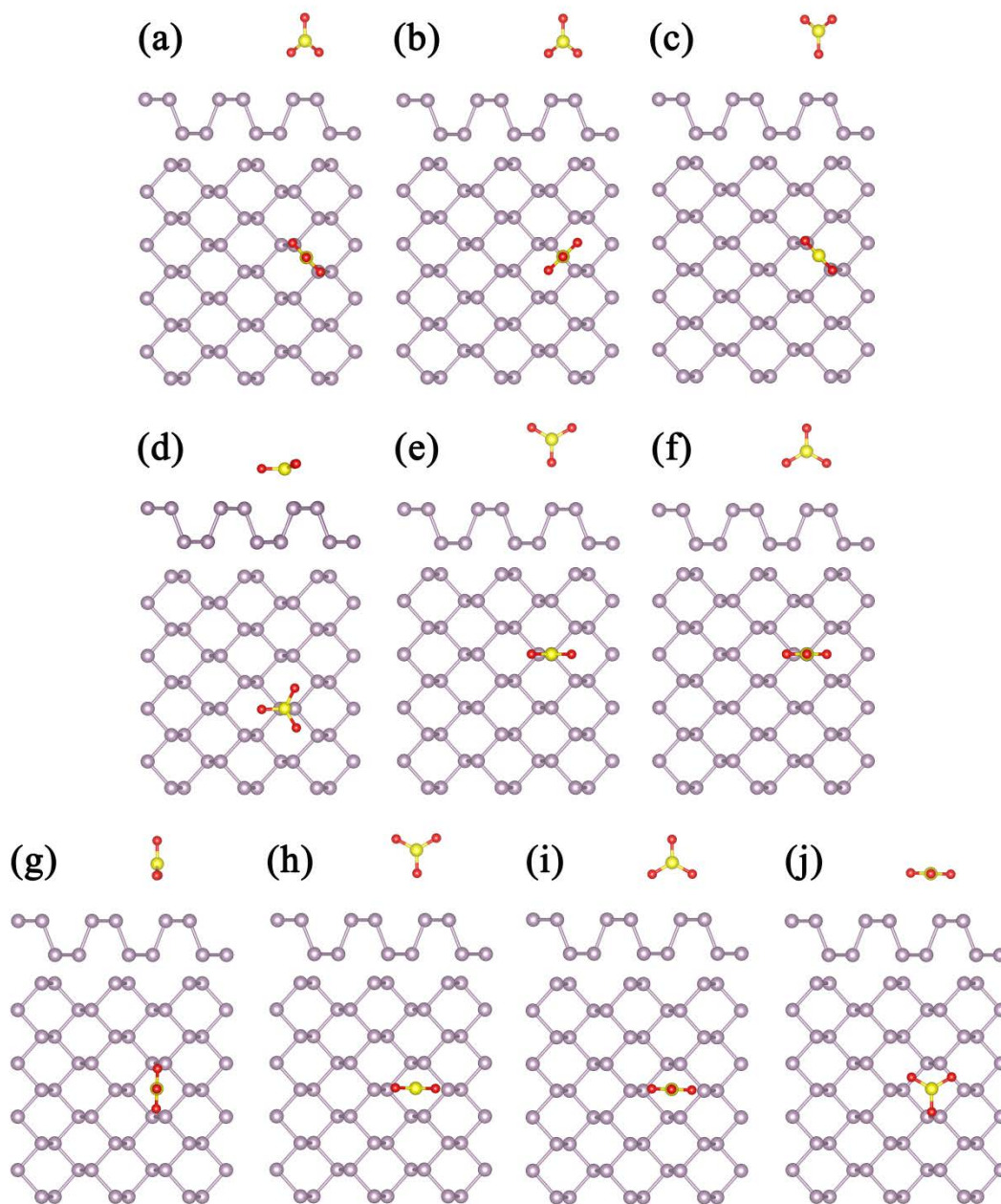


**Figure S1.** The initial structures of  $\text{H}_2\text{S}$  absorbed on  $3 \times 4$  pristine phosphorene in different adsorption sites. (a)~(c) S atoms on bridge sites and H-H lines parallel to phosphorene plane with S atoms towards different directions; (d)-(f) S atoms on top sites and H-H lines 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.



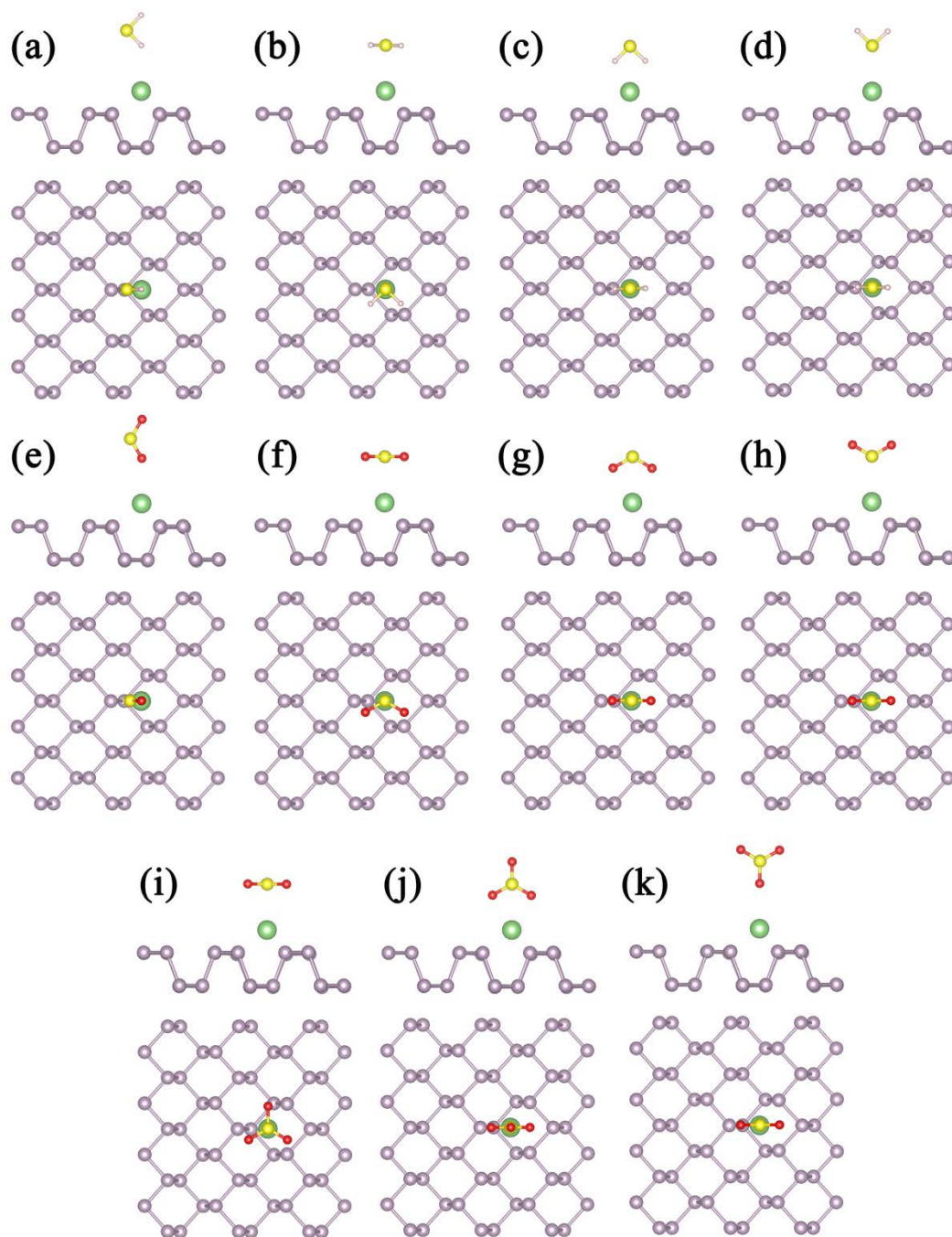
**Figure S2.** The initial structures of  $\text{SO}_2$  absorbed on  $3 \times 4$  pristine phosphorene in different adsorption sites. (a)-(d) S atoms on bridge sites and O-O lines parallel to phosphorene planes with S towards different directions; (f)-(i) S atoms on top sites and O-O lines parallel 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, and O atoms, respectively.

O atoms, respectively.



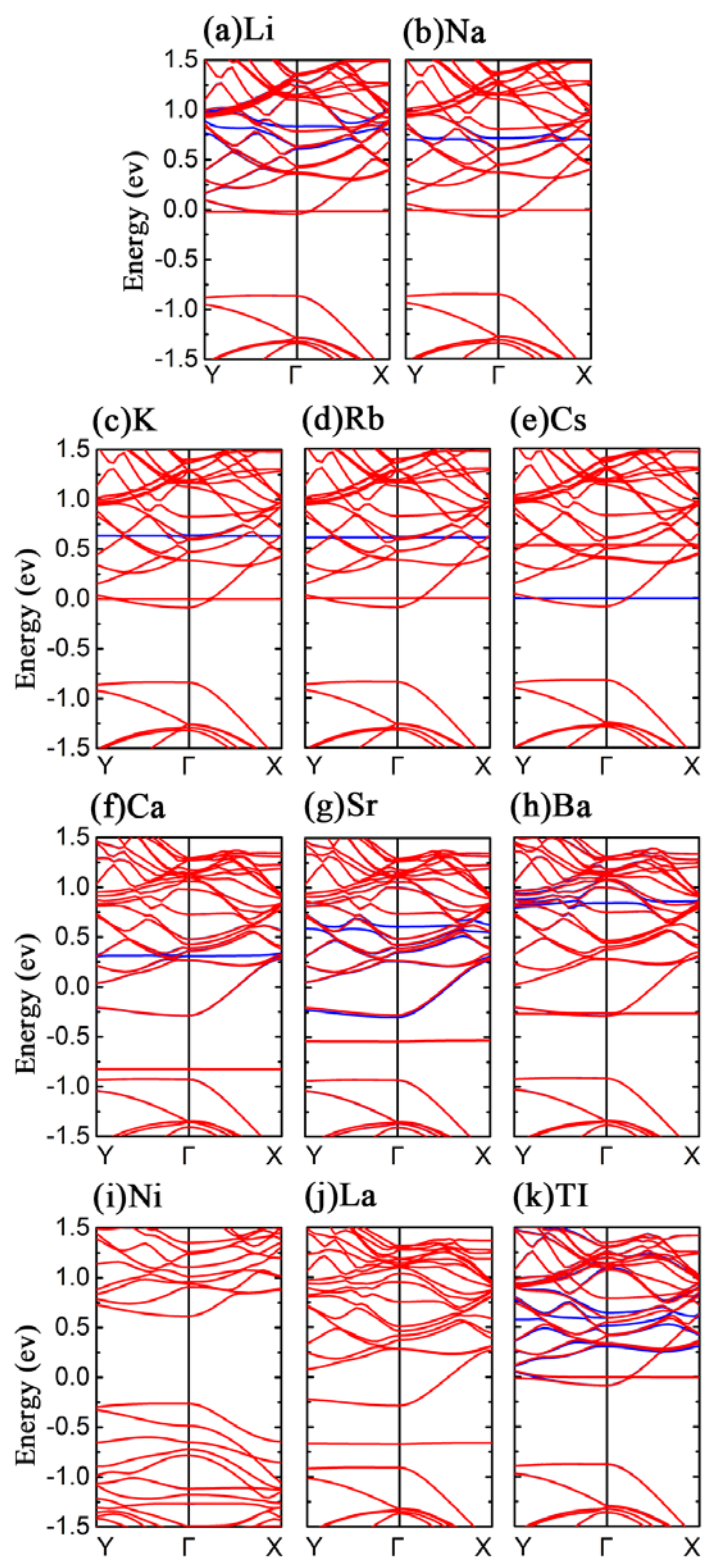
**Figure S3.** The initial structures of  $\text{SO}_3$  adsorbed on  $3 \times 4$  pristine phosphorene in different adsorption sites. S atoms on bridge sites with O-S-O bond angle (a)-(b) toward phosphorene plane and (c) toward outside; S atoms on top sites with (d) O-atomic plane parallel to phosphorene 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.



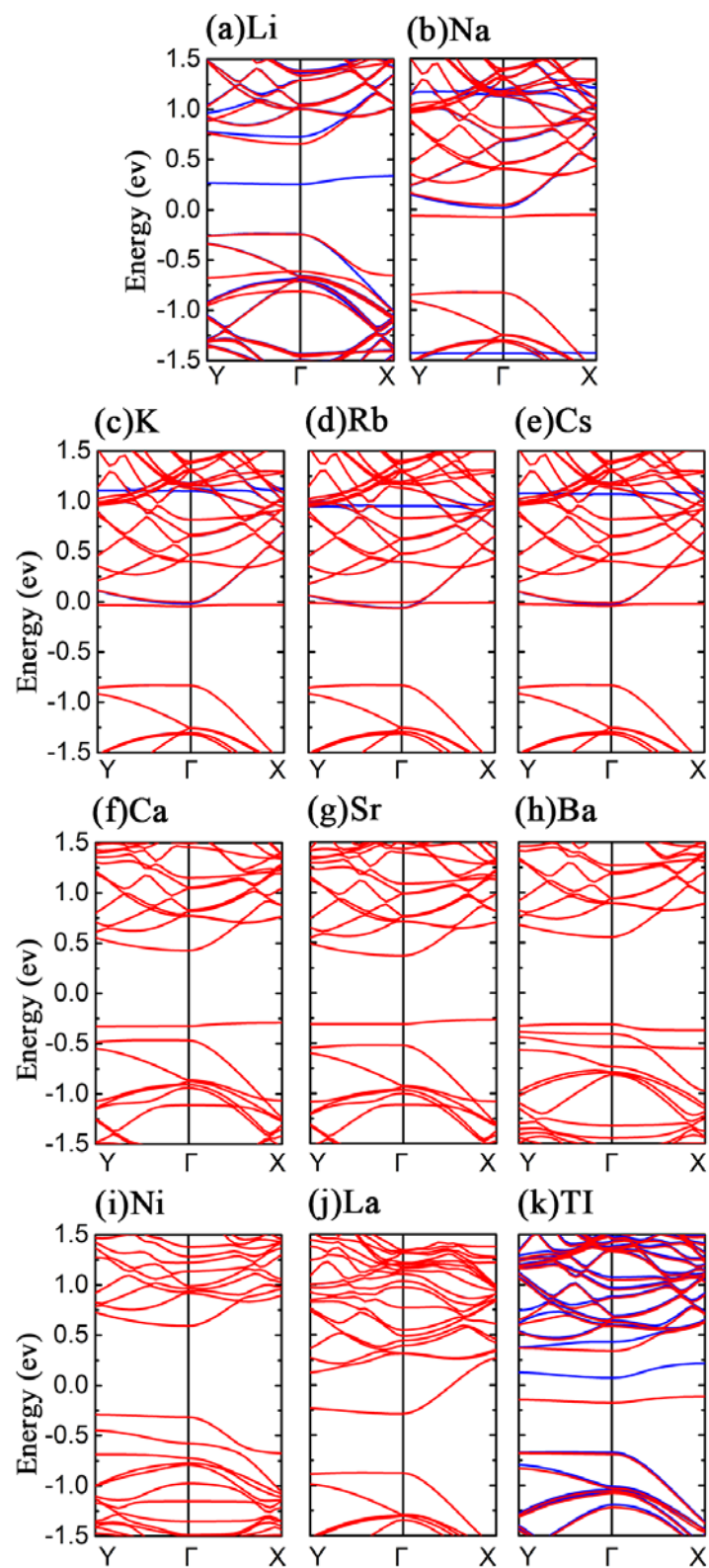


**Figure S4.** The initial structures of (a)-(d)  $\text{H}_2\text{S}$ , (e)-(h)  $\text{SO}_2$ , (i)-(k)  $\text{SO}_3$  absorbed on Li doped phosphorenes. Purple, yellow, white, red and green balls represent P, S, H, O and Li atoms, respectively.

**Figure S5.** The band structures of H<sub>2</sub>S 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<sub>2</sub> 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  $\text{SO}_3$  adsorption on bP-M ( $M=\text{Li, Na, K, Rb, Cs, Ca, Sr, Ba, Ni, La, Tl}$ ). The red and blue curves represent the spin-up and spin-down bands, respectively. The Fermi level is set to zero.