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Supporting Information

Doping MoS_2 monolayer with nonmetal atoms to tune its electronic and magnetic properties as well as chemical activity: a theoretical insight

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Table S1. The computed adsorption energies (eV) of H_2, N_2, O_2, NO, and NO_2 on pristine and doped MoS_2 monolayers by O, B, C, N, and P atoms. [a] the adsorption energy of metal-stable configurations of H_2 and NO_2, [b] the reaction energies (eV) from the meta-stable configurations of H_2 and NO_2 to the most stable configurations.

	H_2	N_2	O_2	NO	NO_2
pristine MoS_2	-0.10	-0.14	-0.12	-0.18	-0.20
O-MoS_2	-0.14	-0.20	-0.17	-0.26	-0.28
B-MoS_2	-0.11[a]/-1.19[b]	-1.48	-1.92	-3.36	-2.16[a]/-1.07[b]
C-MoS_2	-0.15[a]/-1.93[b]	-1.28	-1.08	-2.32	-1.88[a]/-0.50[b]
N-MoS_2	-0.16	-0.22	-0.36	-1.61	-0.90[a]/-0.59[b]
P-MoS_2	-0.10	-0.14	-0.75	-0.11	-1.54[a]/-0.63[b]

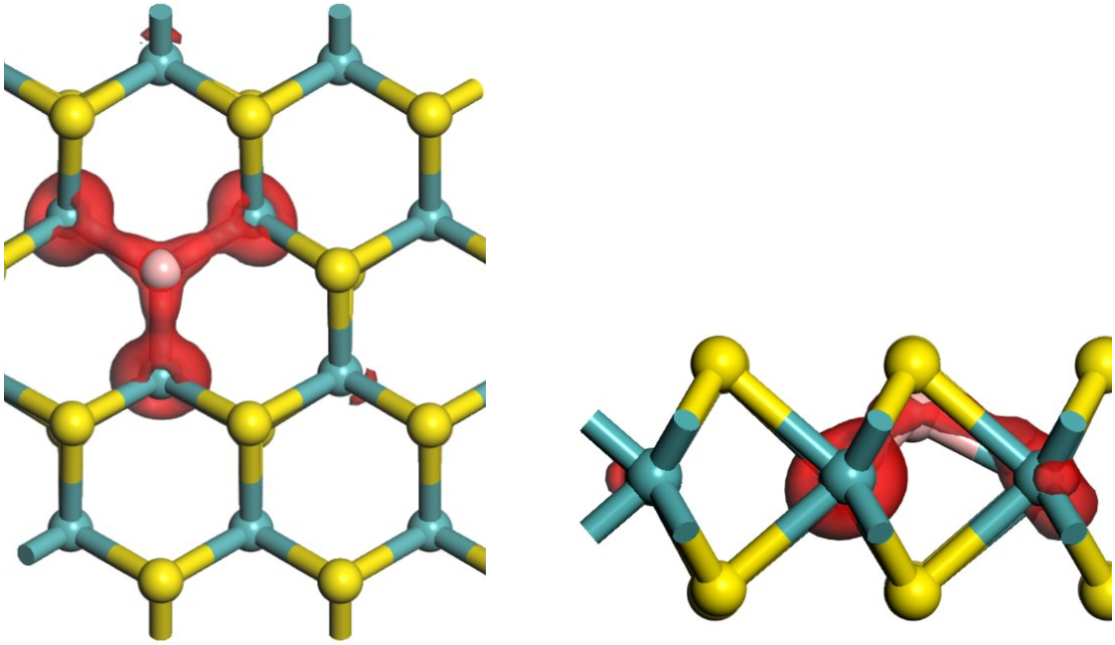

Figure S1. The computed spin density of B-doped MoS_2 nanosheet. The isosurface value is 0.01 electrons/a.u.^{3}.

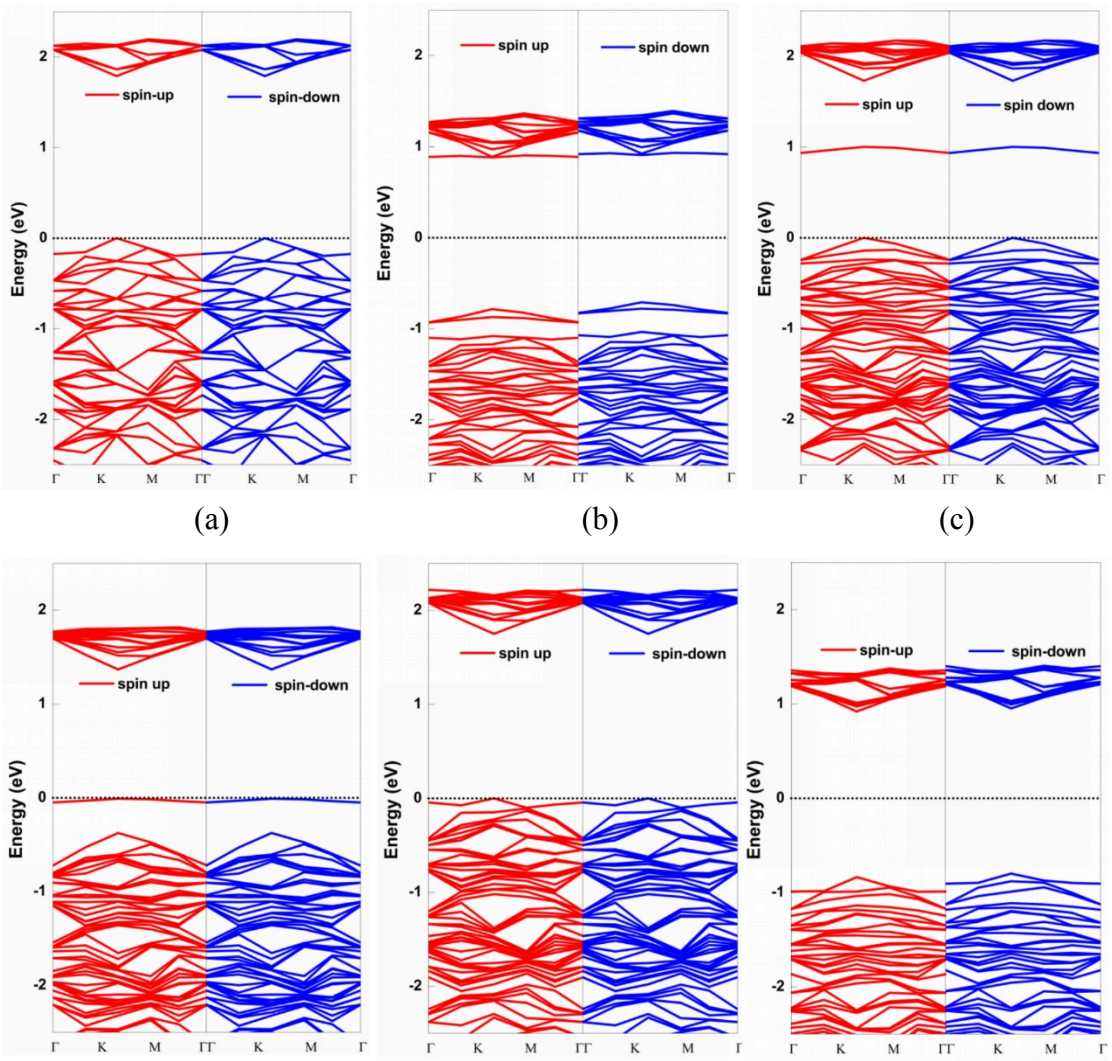

Figure S2. The computed band structures of (a) pristine and nonmetal doped MoS_2 nanosheets with (b) B, (c) C, (d) N, (e) P, and (f) O atoms. The Fermi level was set zero in dotted lines.

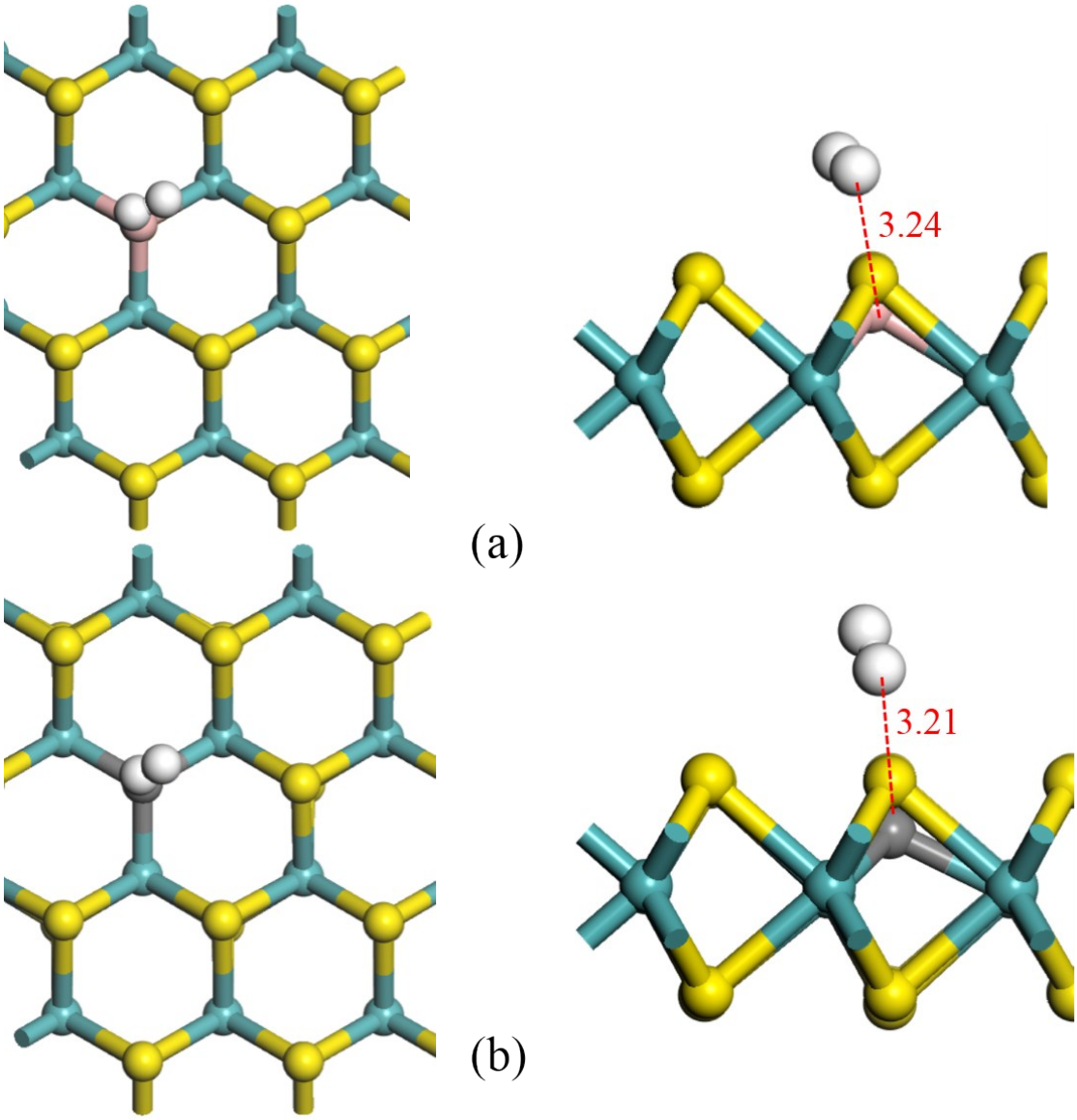

Figure S3. H_2 physisorption on (a) B- and (b) C-doped MoS_2 monolayers.

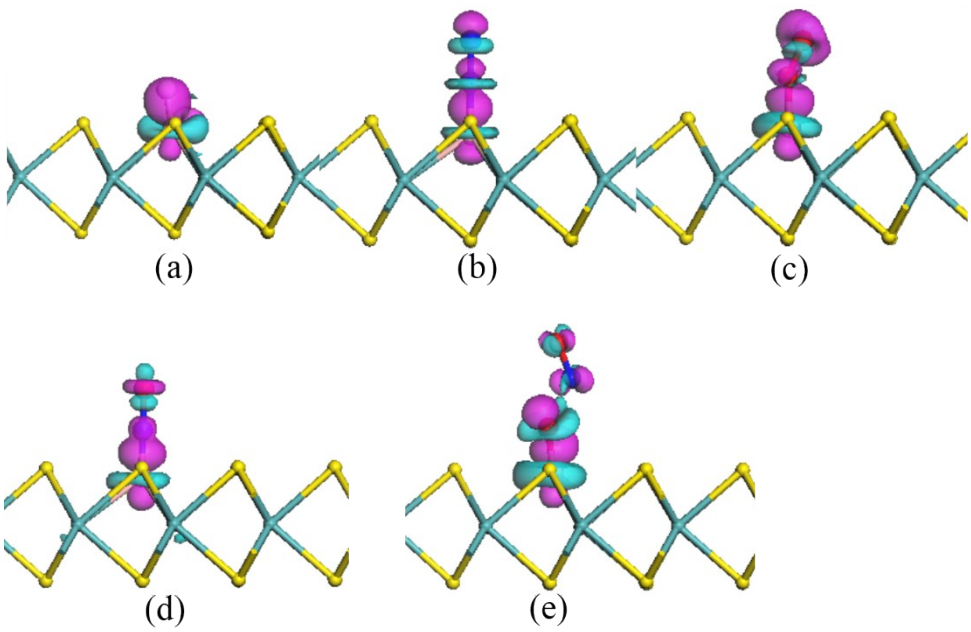

Figure S4. The computed charge difference density of (a) H_2, (b) N_2, (c) O_2, (d) NO, and (e) NO_2 molecules adsorbed on B-doped MoS_2 nanosheet. Regions of electron accumulation and depletion are displayed in pink and cyan, respectively. The isosurface value is ±0.05 electrons/a.u^3.

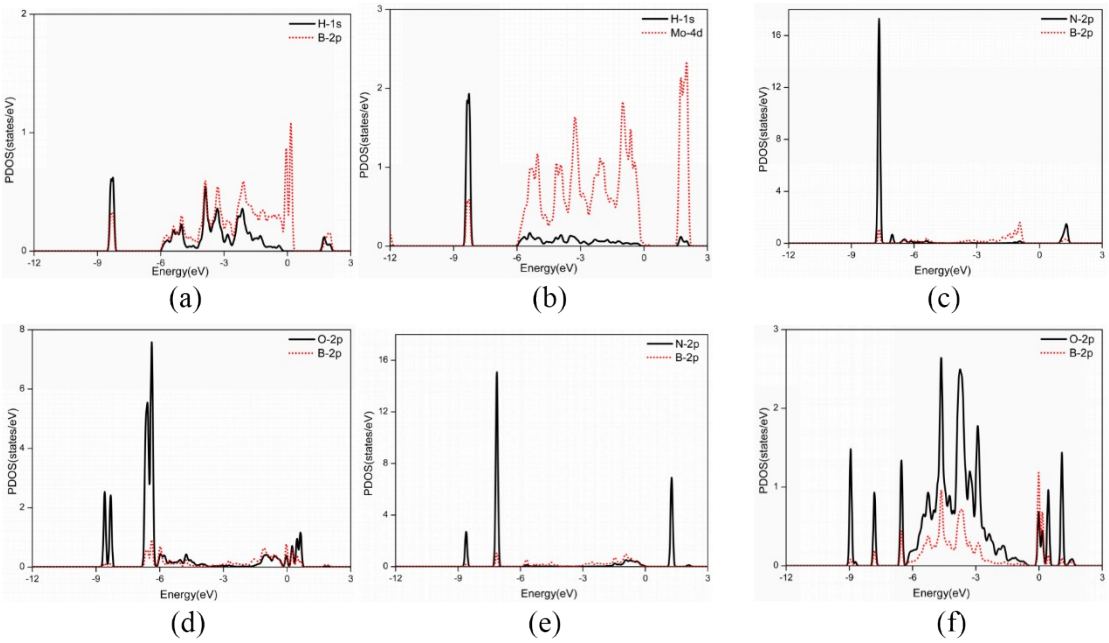

Figure S5. The computed projected density of states (PDOSs) of (a) H_2 (H on B), (b) H_2 (H on Mo), (c) N_2, (d) O_2, (e) NO, and (f) NO_2 molecules adsorbed on B-doped MoS_2 monolayer.

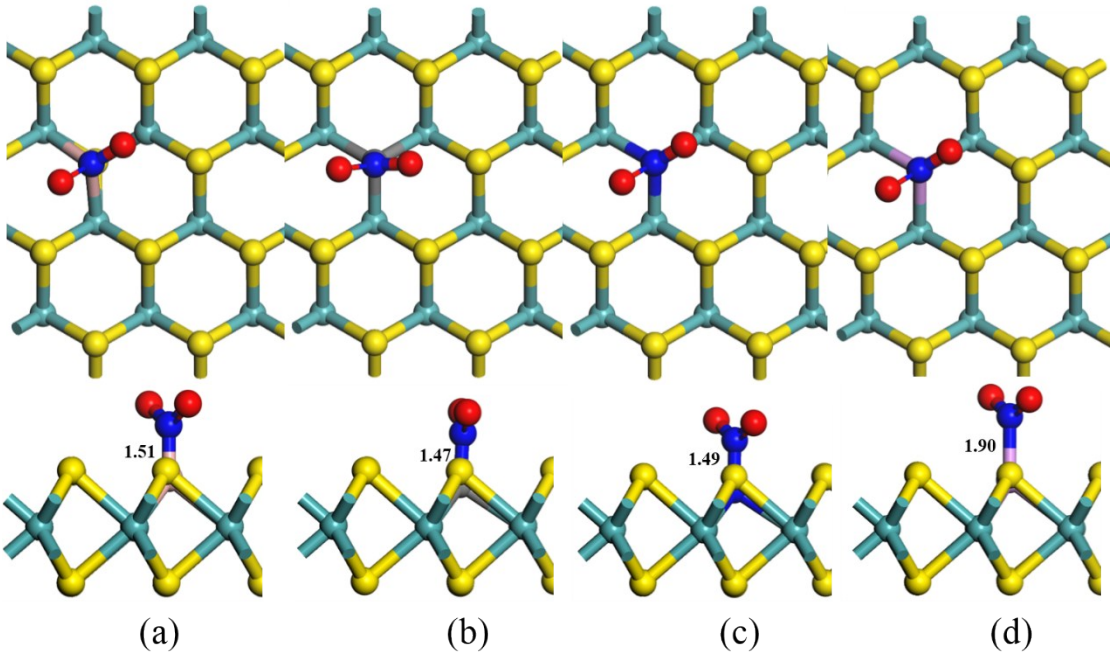

Figure S6. The top and side views of the meta-stable configurations for NO_2 molecule adsorption on (a) B-, (b) C-, (c) N-, and (d) P-doped MoS_2 monolayers.

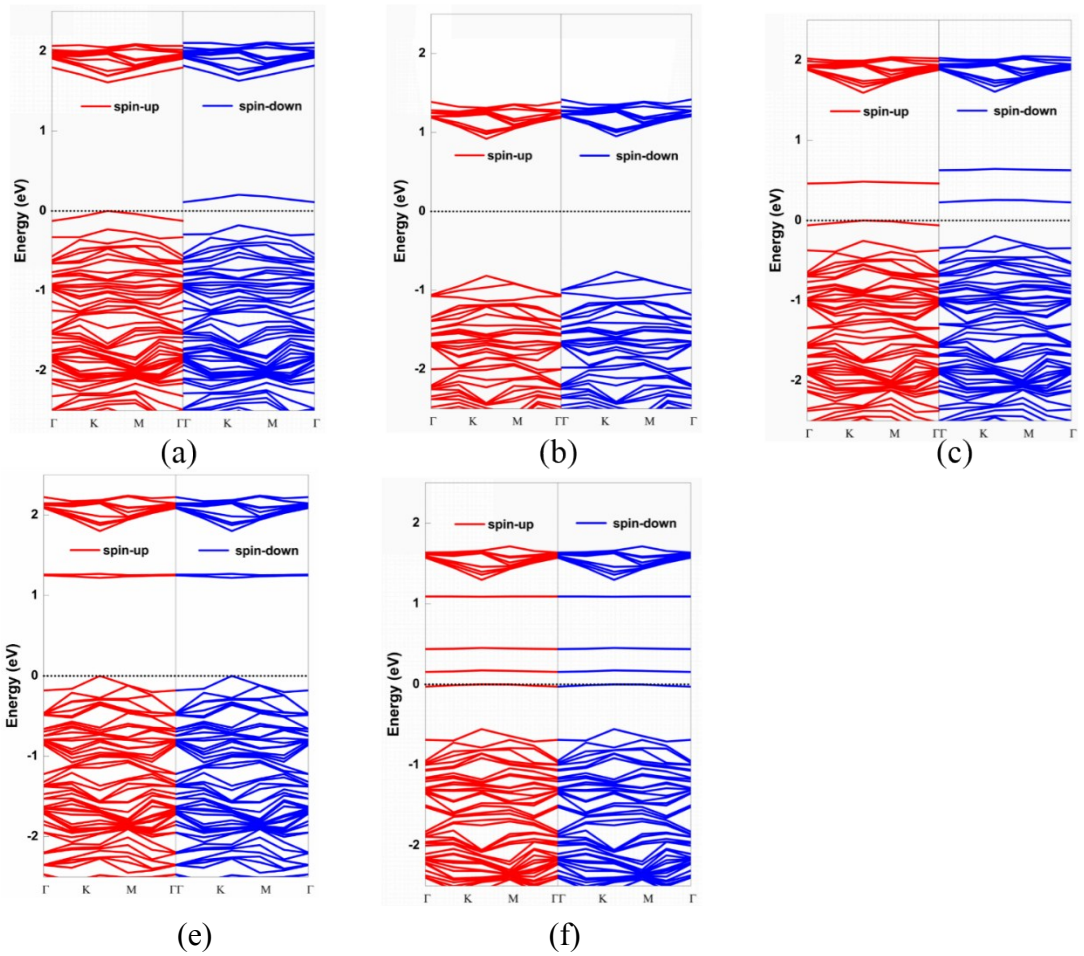

Figure S7. The computed band structures of B-doped MoS_2 monolayer adsorbed by (a) H_2, (b) N_2, (c) O_2, (d) NO, and (e) NO_2 molecules. The Fermi level was set zero in dotted lines.

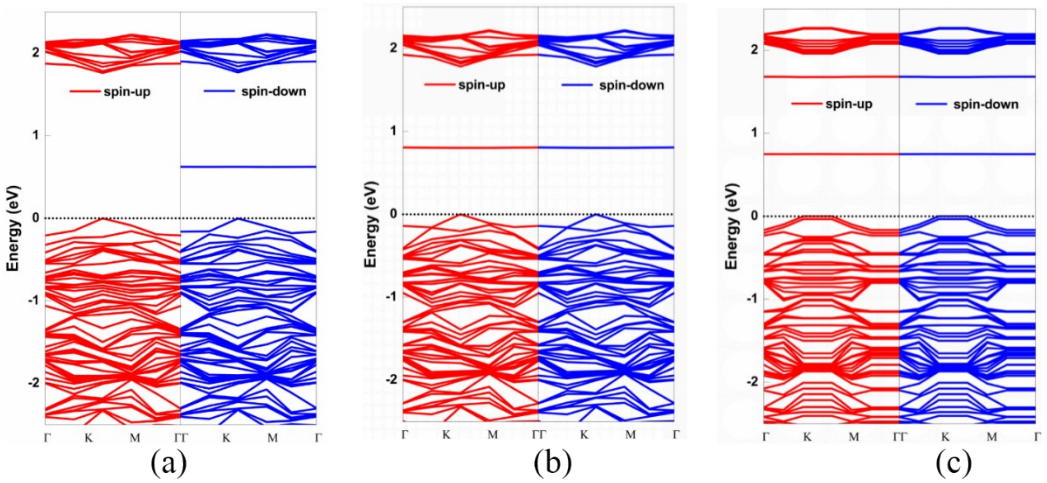

Figure S8. The computed band structures of P-doped MoS_2 monolayer adsorbed by (a) O_2, (b) NO, and (c) NO_2 molecules. The Fermi level was set zero in dotted lines.

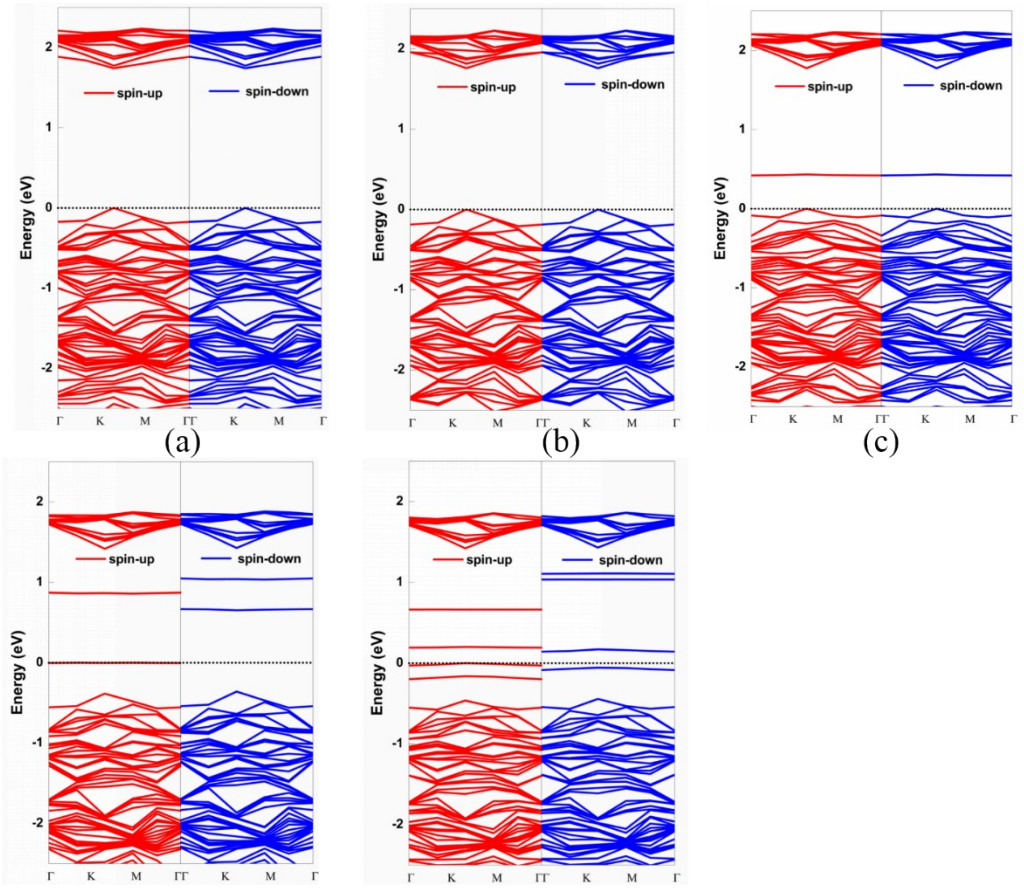

Figure S9. The computed band structures of C-doped MoS_2 monolayer adsorbed by (a) H_2, (b) N_2, (c) O_2, (d) NO, and (e) NO_2 molecules. The Fermi level was set zero in dotted lines.

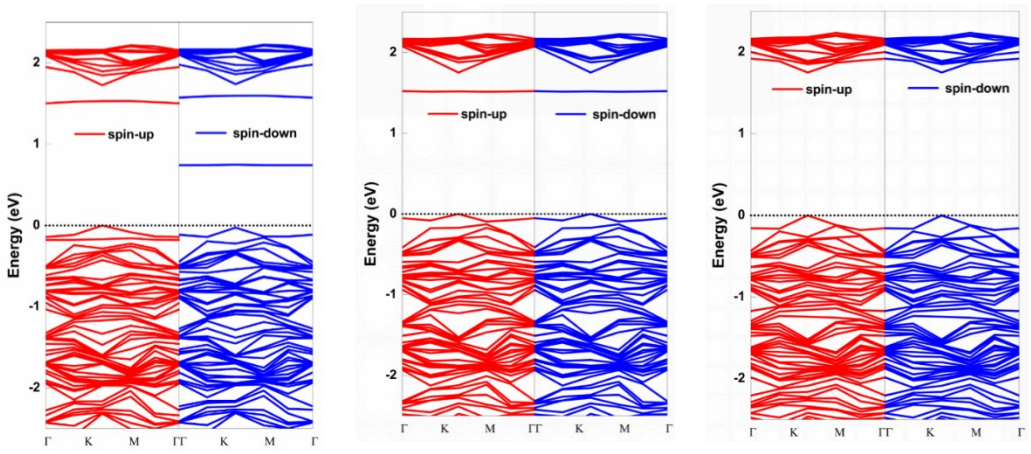

Figure S10. The computed band structures of N-doped MoS_2 monolayer adsorbed by (a) O_2, (b) NO, and (c) NO_2 molecules. The Fermi level was set zero in dotted lines.