Inorganic molecules (O2, NO) adsorption on Nitrogen and Phosphorus doped MoS_2 monolayer using first principle calculations

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Table S1. Adsorption energy (E_{ad}) of the O_2 gas molecule to the N and P substituted (4×4) MoS_2 monolayer for different configurations, P, V represents parallel and vertical orientations of the molecule, respectively.

Configuration	Absorbent	Absorbate	Ead (eV)[a]	Erel (eV)[b]
P_1	N-MoS_2	O_2	-0.32	0.00
V_1	N-MoS_2	O_2	-0.29	0.03
P2	N-MoS_2	O_2	1.67	1.99
P_1	P-MoS_2	O_2	-1.27	0.00
V1	P-MoS_2	O_2	-1.11	0.16
P2	P-MoS_2	O_2	-0.80	2.07

[a] The adsorption energy per gas molecule to the MoS_2 surface.

[b] Relative energy defined as the total energy of each configuration minus that of the most stable configuration A_i.

Table S2. Adsorption energy (E_{ad}) of NO gas molecule to the N and P substituted (4×4)MoS_2 monolayer for different configurations, P, V represents parallel and vertical orientations of the molecule, respectively.

Configuration	Absorbent	Absorbate	Ead (eV)[a]	Erel (eV)[b]
P_1	N-MoS_2	NO	-0.56	0.00
V_1	N-MoS_2	NO	-0.46	0.09
P2	N-MoS_2	NO	-0.09	0.47
P_1	P-MoS_2	NO	-1.44	0.00
V_1	P-MoS_2	NO	-1.42	0.01
P_2	P-MoS_2	NO	-0.64	0.79
P_3	P-MoS_2	NO	-0.36	1.07

[a] The adsorption energy per gas molecule to the MoS_2 surface.

[b] Relative energy defined as the total energy of each configuration minus that of the most stable configuration

Table S3. Relative energy of substituted (4 × 4) MoS_2 monolayer for different configurations, respectively.

Configuration	Dopant	Erel (eV)b
A	N	0.00
B	N	0.005
C	N	0.05
D	N	0.36
A	P	0.00
B	P	0.37
C	P	0.40
D	P	0.43

[a] The substituted Nitrogen and phosphorus atoms.

[b] Relative energy defined as the total energy of each configuration minus that of the most stable configuration

Tables S3 compares the relative stabilities of various configurations of the doped (4×4) MoS_2 monolayer and doping concentration ranges from 3.12% to 6.25% per MoS_2 unit, corresponding to N_D= 1-2, here N_D represents the number of impurity atoms. In this regard, we note that MoS_2 layer contains three sublayers, and impurities can only be entered in the upper and lower sublayers (U_U, U_L) occupied by sulfur atoms. Here, U_U and U_L denote the upper and lower sublayers of the MoS_2 layer, respectively. For N_D = 1 value, the impurity atom doped into the center of the MoS_2 monolayer and model ensure that distance among the adjacent image is larger than 12.0 Å. However, for N_D = 2 in configuration A, B impurity atom doped on U_U and other on U_L sublayers of the MoS_2 monolayer far away from the central atom to avoid interaction between the dopants and one S-Mo bond apart as shown in Fig. S1. On the other hand, in configuration C and D second impurities located on U_U sublayer of the MoS_2 are two and four S-Mo bonds apart from a central atom. The most stable configuration is referred to as A and it is more stable than the B, C, and D, irrespective of N_D. We used a most stable configuration in this work to study the adsorption of gas molecules. Based on this observation, configurations with higher defects concentrations can be generated in such a way to include as many S-Mo motifs as possible.

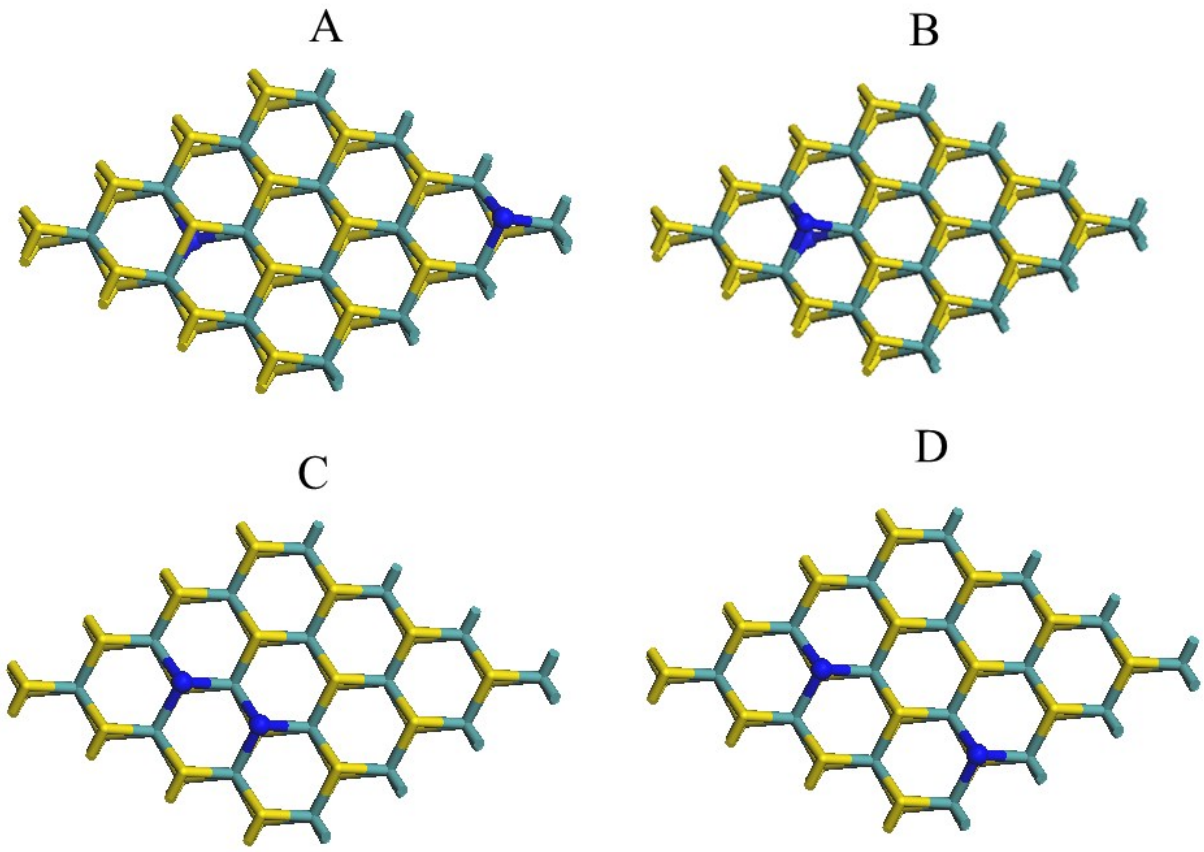

Fig. S1. The chemical structure for a different configuration of $(4 \times 4)MoS_2$ monolayer substituted with N atom, violet, yellow, and green sphere represent Mo, S, and N atoms, respectively.

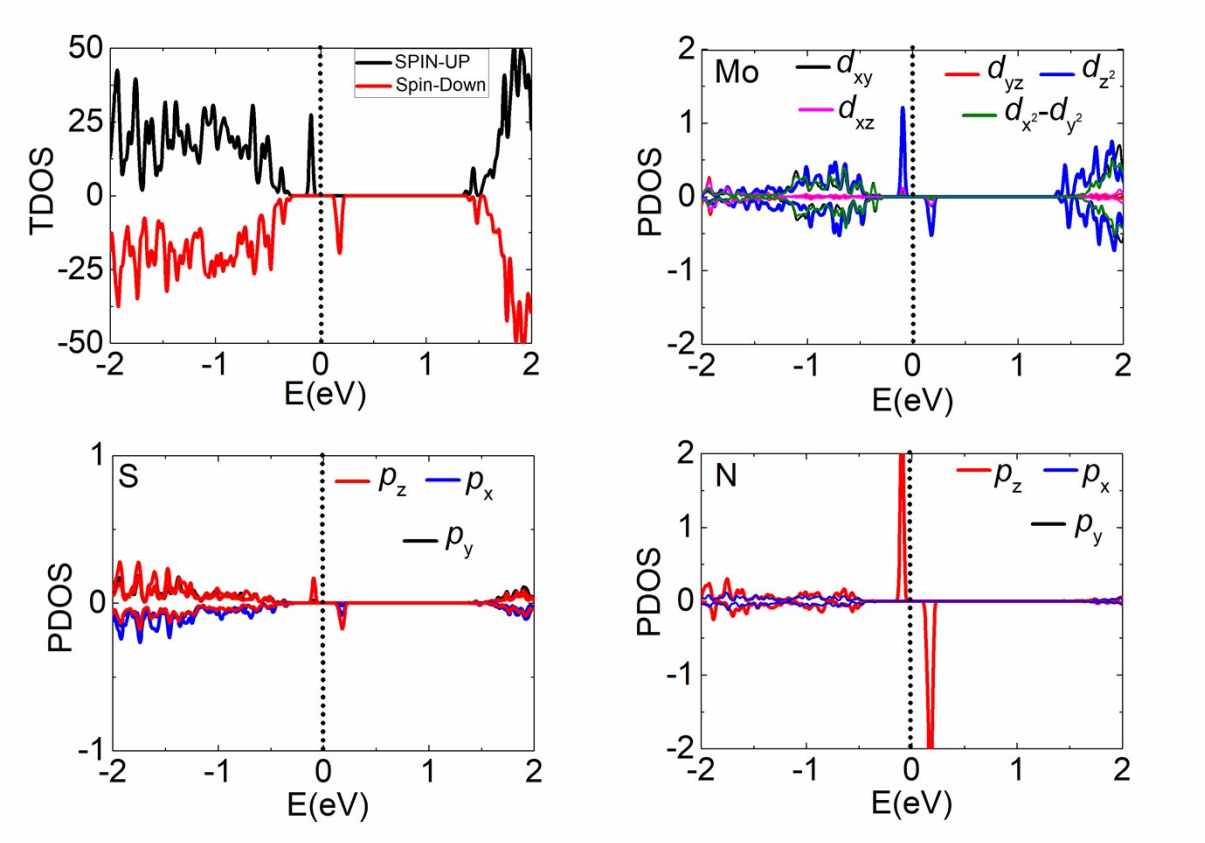

Fig. S2. The total electronic density of states (TDOS) of (4 × 4)N-MoS_2 monolayer and their corresponding PDOS of Mo, S, and N atoms for a spin-up and spin-down states, respectively.

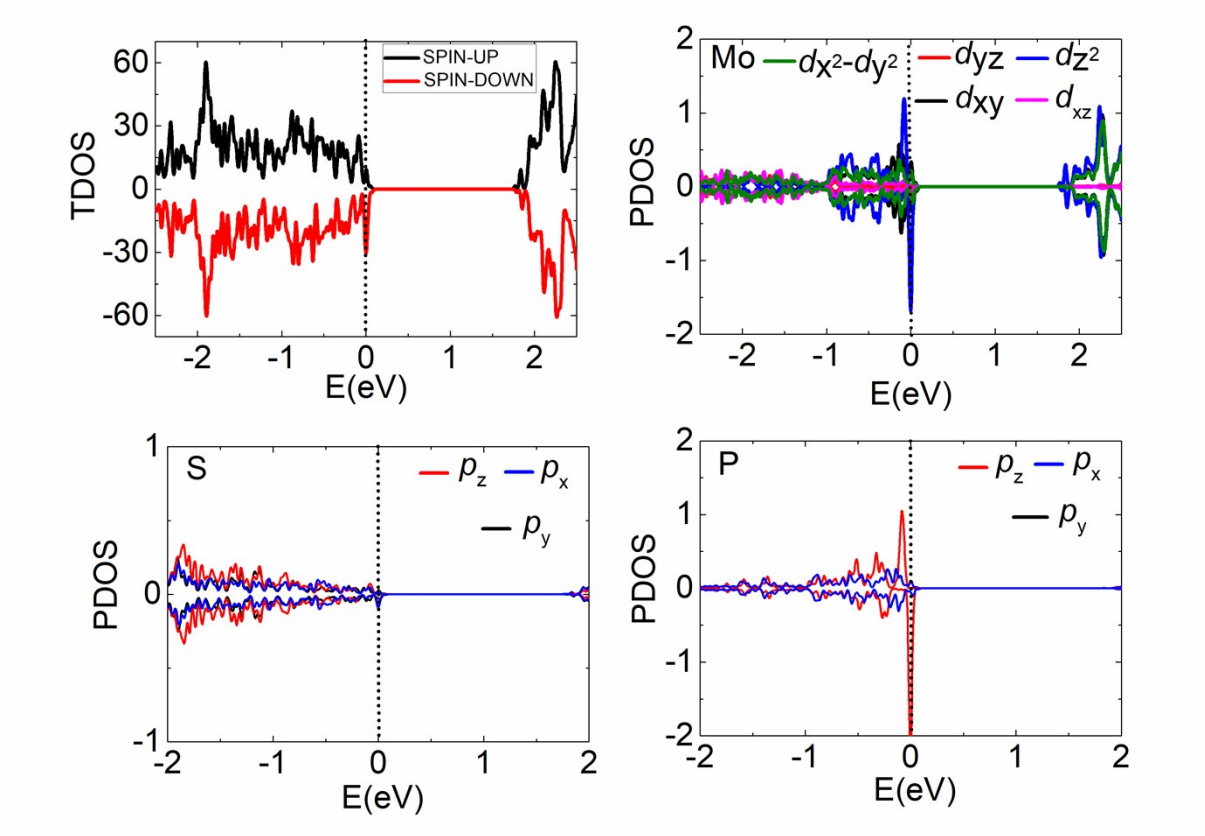

Fig. S3. The total electronic density of states (TDOS) of (4 × 4)P-MoS_2 monolayer and their corresponding PDOS of Mo, S, and P atoms for a spin-up and spin-down states, respectively.

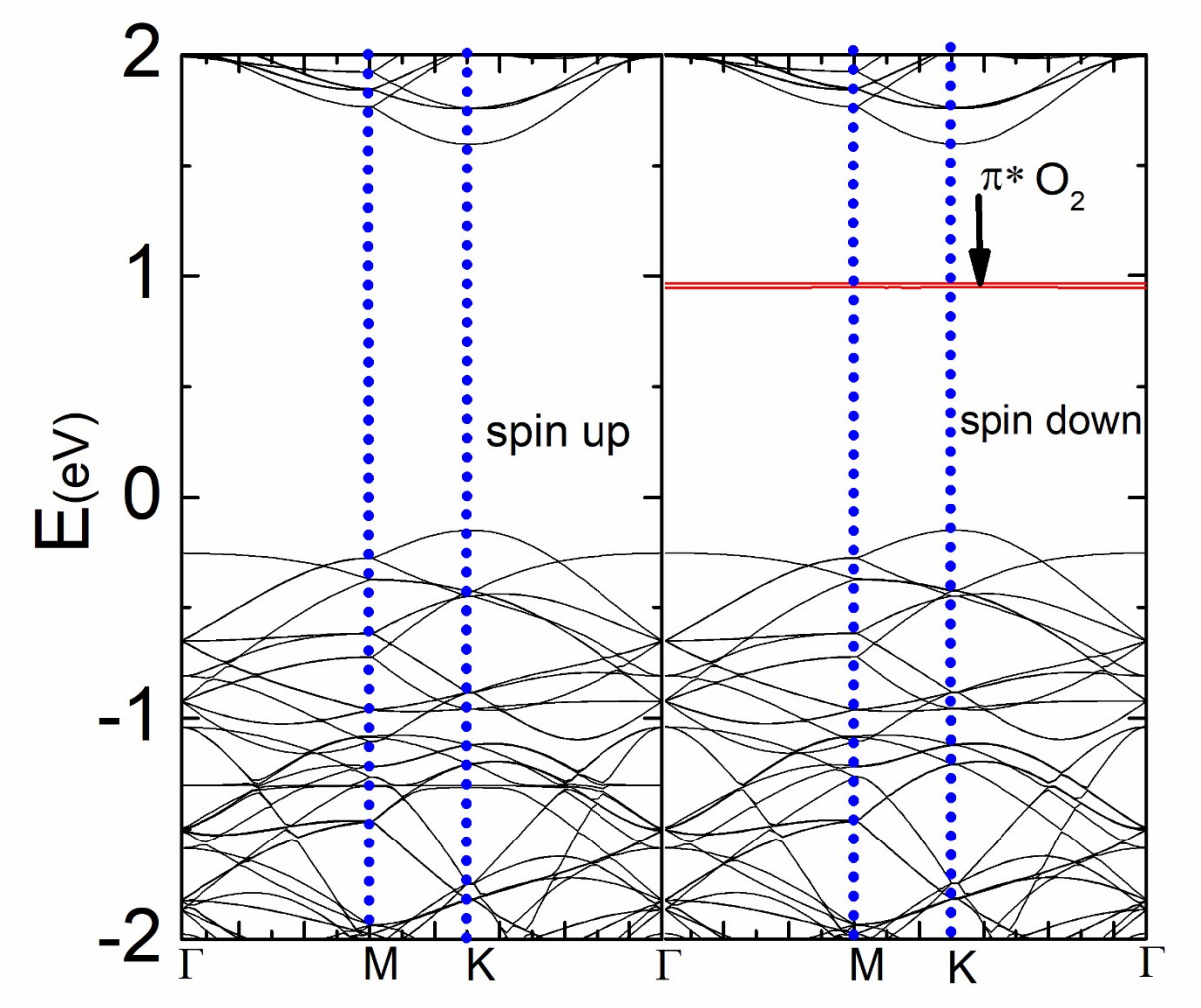

Fig. S4. Band structure of a $(4 \times 4)MoS_2$-O_2 complex system for spin-up and spin-down states, respectively.

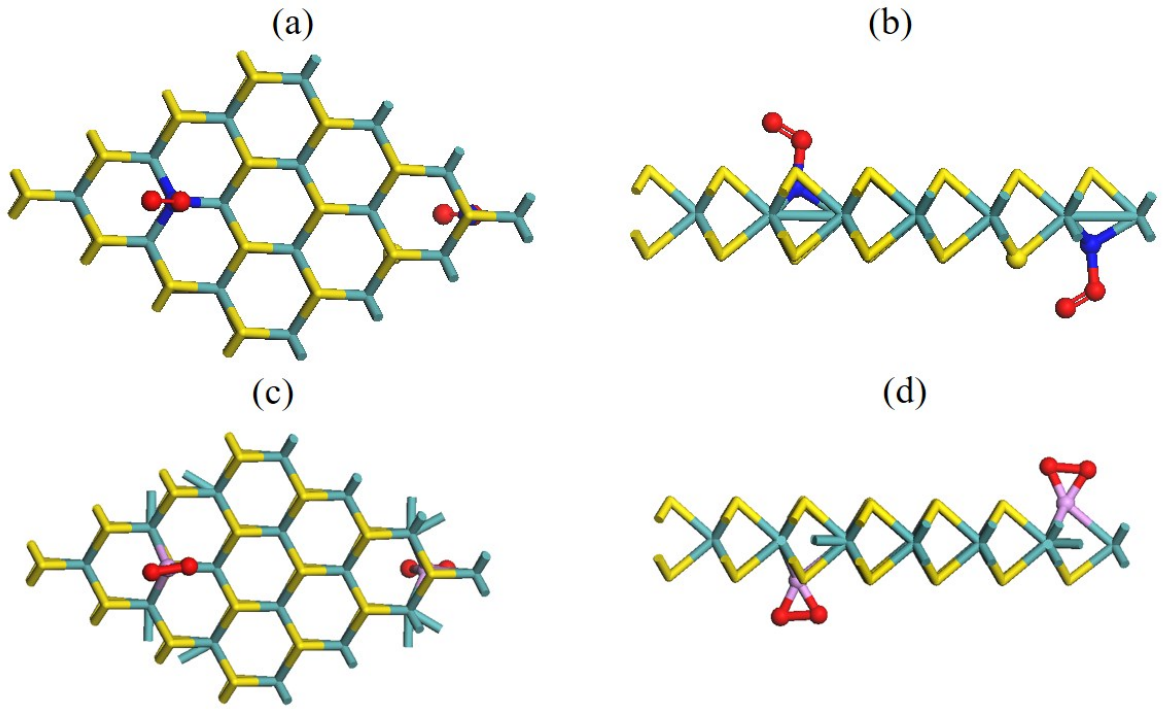

Fig. S5. Top (a,c) and side (b,d) view for the chemical structure of the 2N and 2P substituted MoS_2-O_2 complex, violet, yellow, green, red and purple sticks represent Mo, S, N, O and P atoms, respectively.

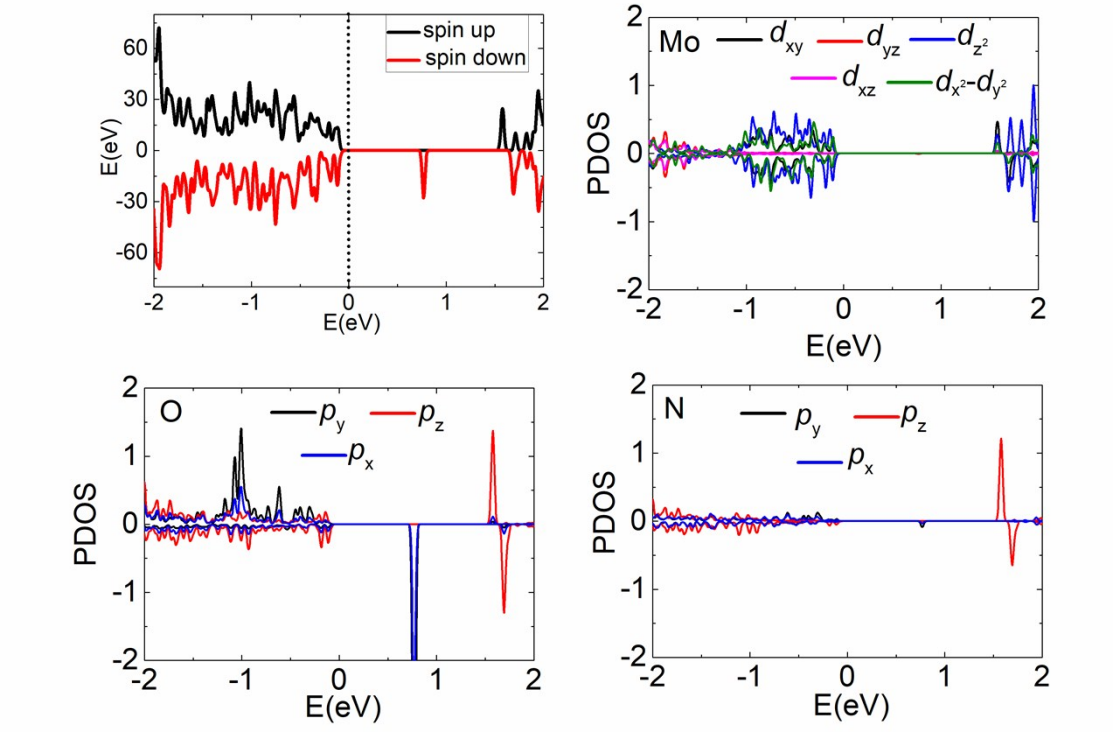

Fig. S6. The total electronic density of states (TDOS) of the (4 × 4)N-MoS_2-O_2 complex system and their corresponding PDOS of Mo, N, and O atoms for a spin-up and spin-down states, respectively.

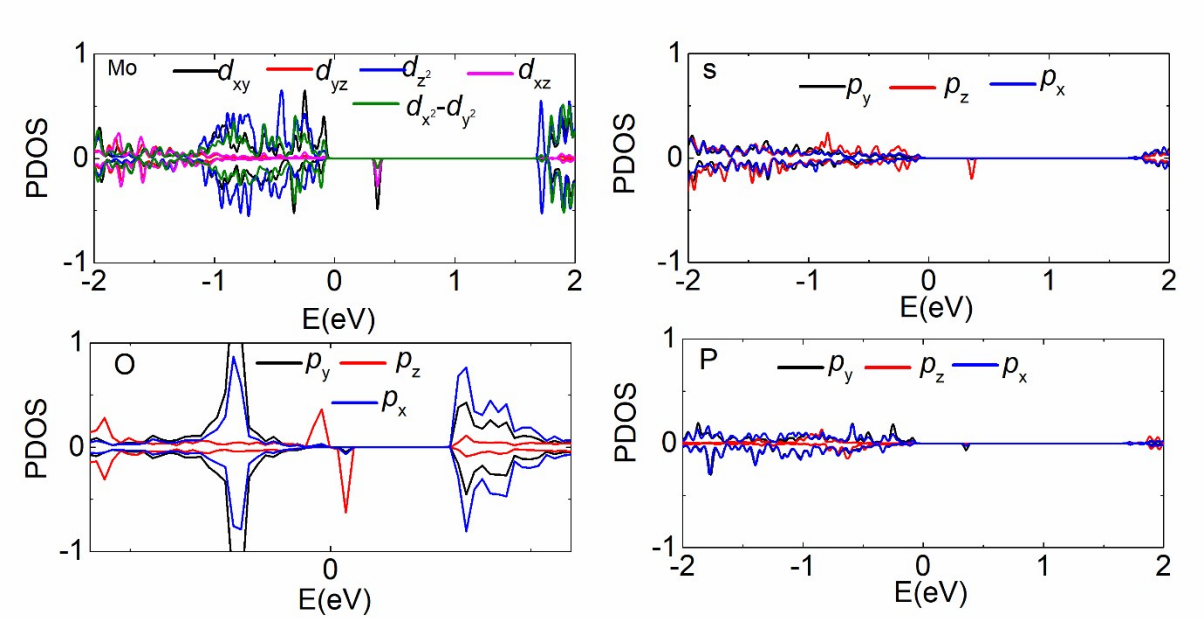

Fig. S7 The (PDOS) of (4 × 4)P-MoS_2-O_2 complex corresponding Mo, S, P, and O atoms for a spin-up and spin-down states, respectively.

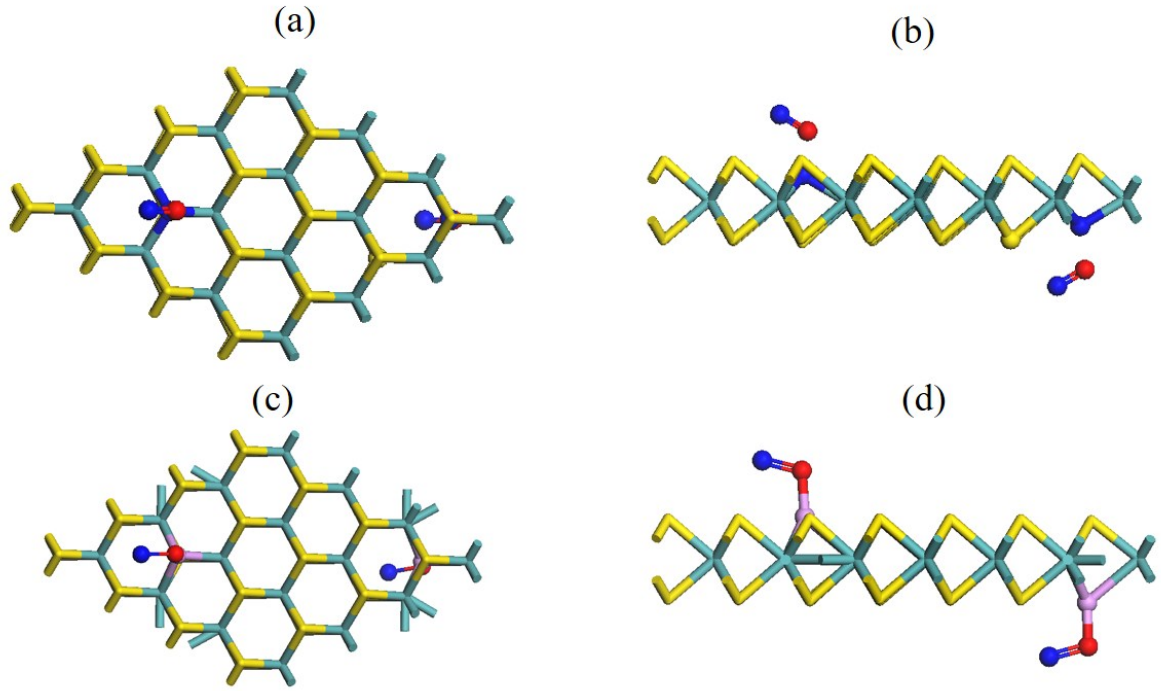

Fig. S8 Top (a,c) and side (b,d) view for a chemical structure of the 2N and 2P substituted MoS_2-NO complex, violet, yellow, green, red and purple sticks represent the Mo, S, N, O and

P atoms, respectively.

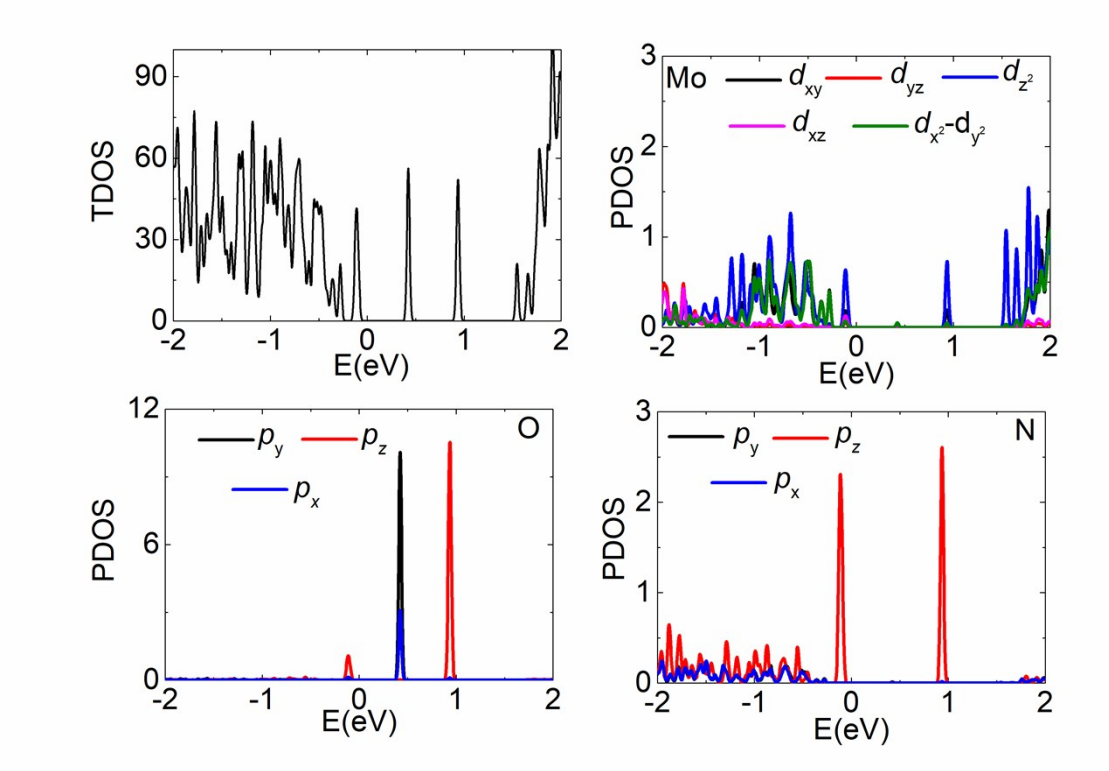

Fig. S9. The total electronic density of states (TDOS) of (4 × 4)N-MoS_2-NO complex and their corresponding PDOS of Mo, N, and O atoms, respectively.

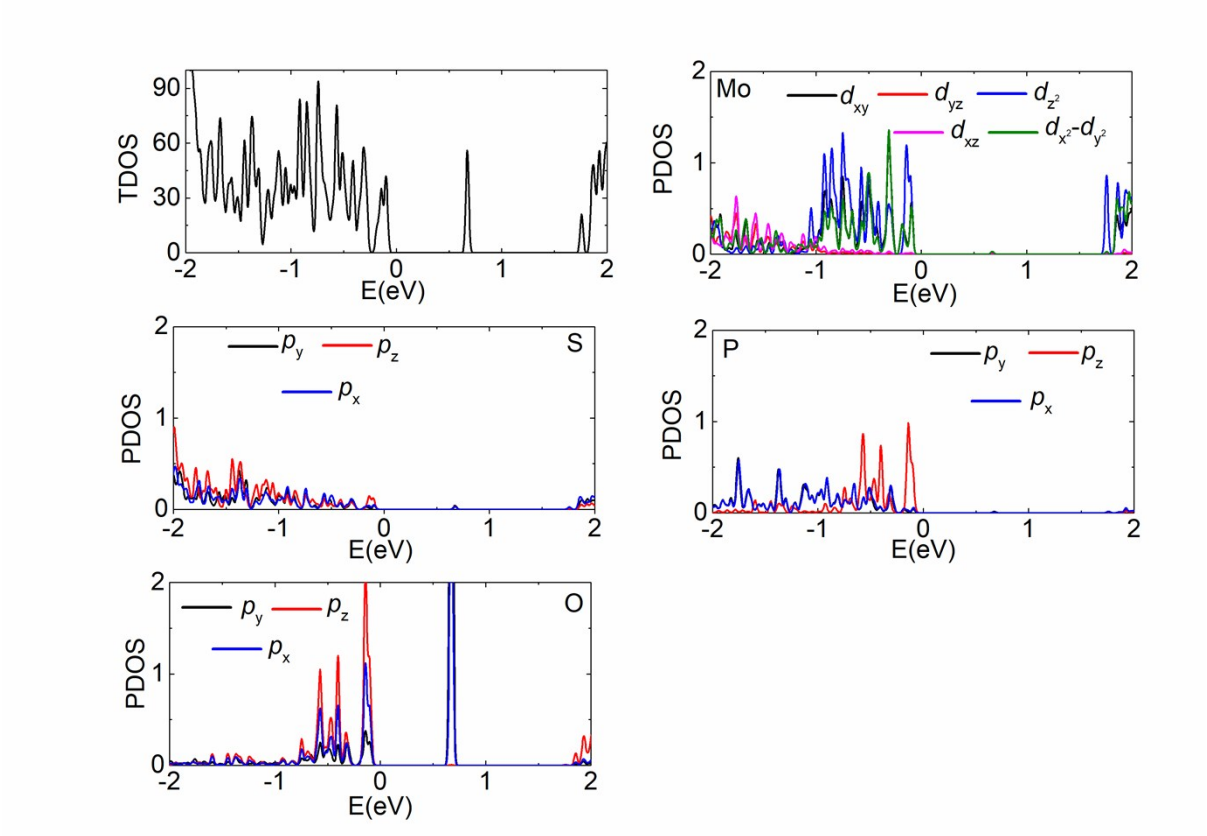

Fig. S10 The total electronic density of states (TDOS) of (4 × 4)P-MoS_2-NO complex and their corresponding PDOS of Mo, S, P, and O atoms, respectively.