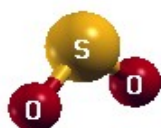


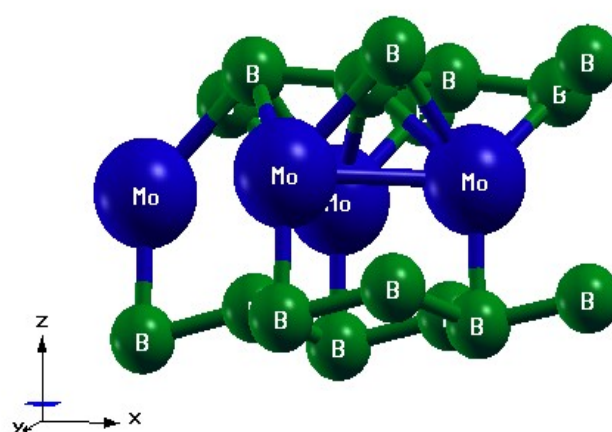
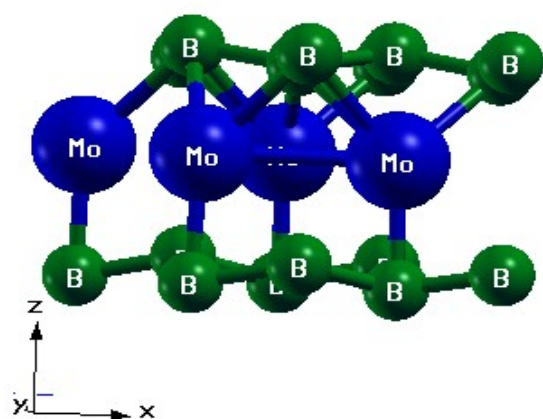
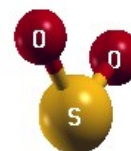
Supplementary Information

“An Ab-initio Study of Sensing Applications of MoB₂ Monolayer: A Potential Gas Sensor.”

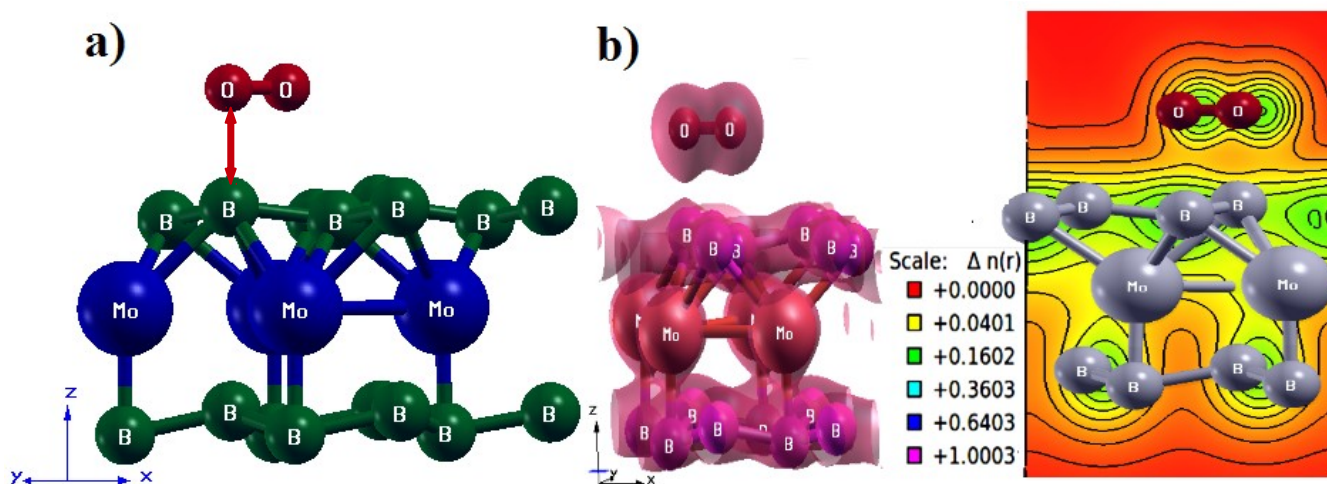
a) S-up



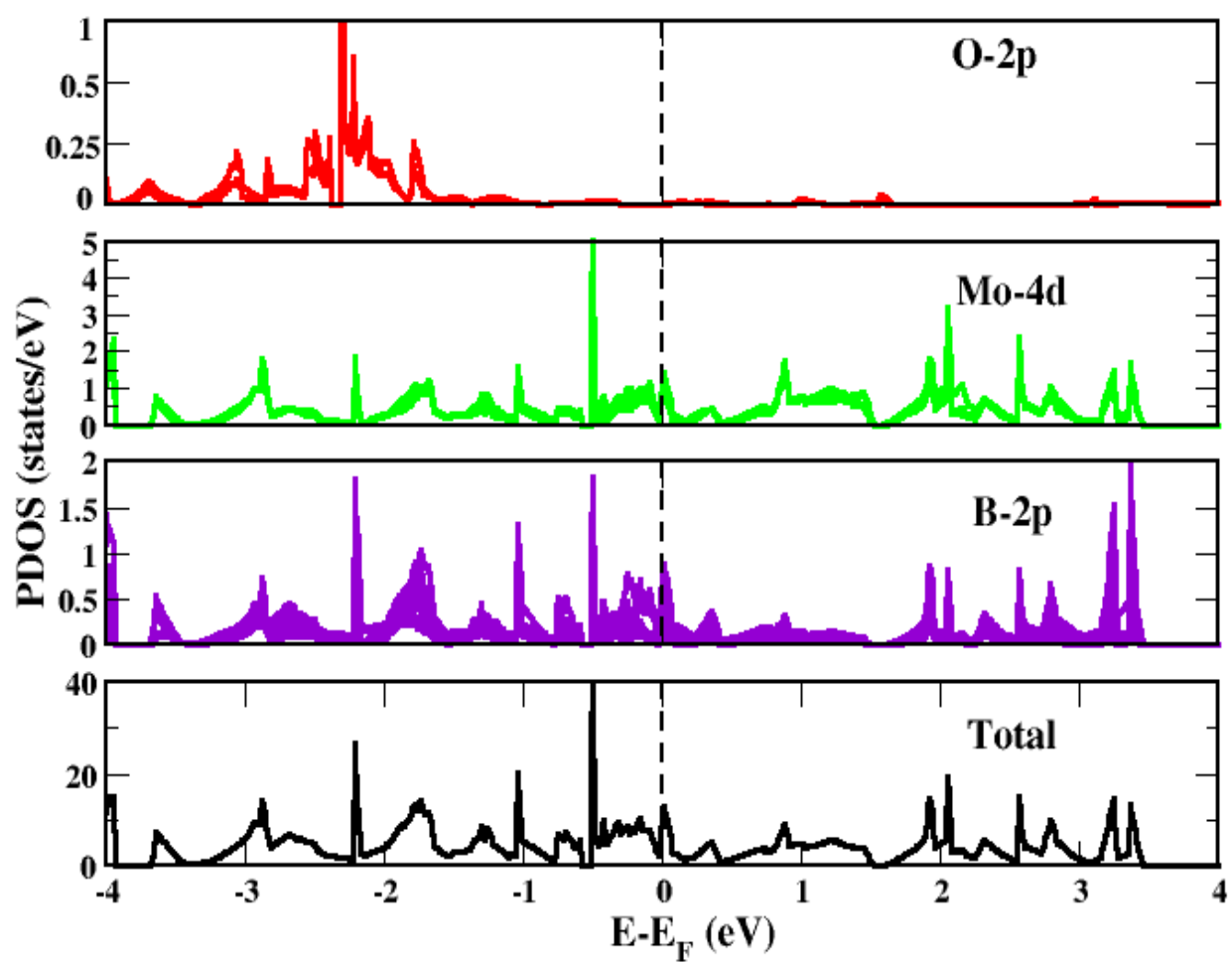
b) S-down



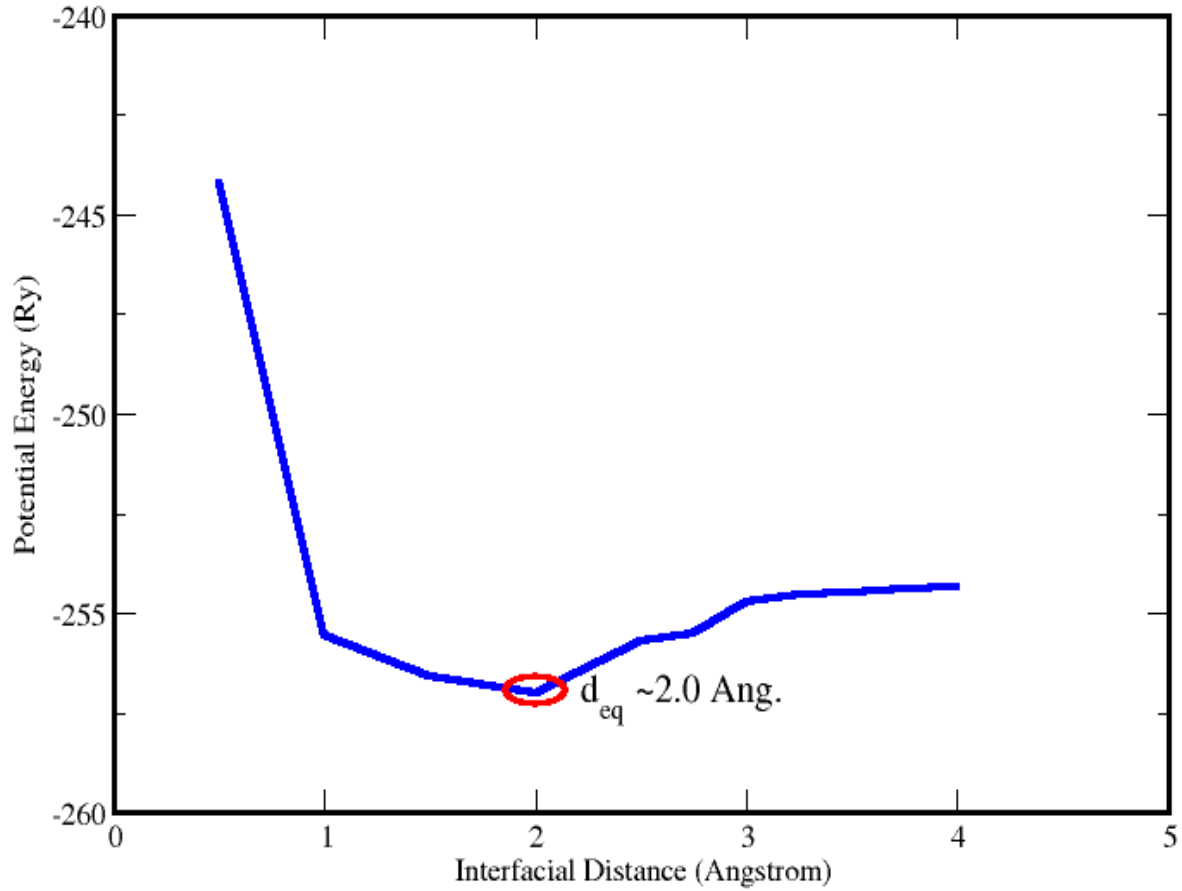
Supplementary Figure 1: SO₂ gas molecule placed over MoB₂ monolayer showing a) S-up and b) S-down configuration.



Supplementary Figure 2: a) O₂ gas molecule placed over MoB₂ monolayer; [Note- Red double sided arrow indicates the interfacial distance $d_{eq} \sim 2.0 \text{ \AA}$] and b) Charge dispersion schematics for O₂ gas molecule over MoB₂ monolayer.



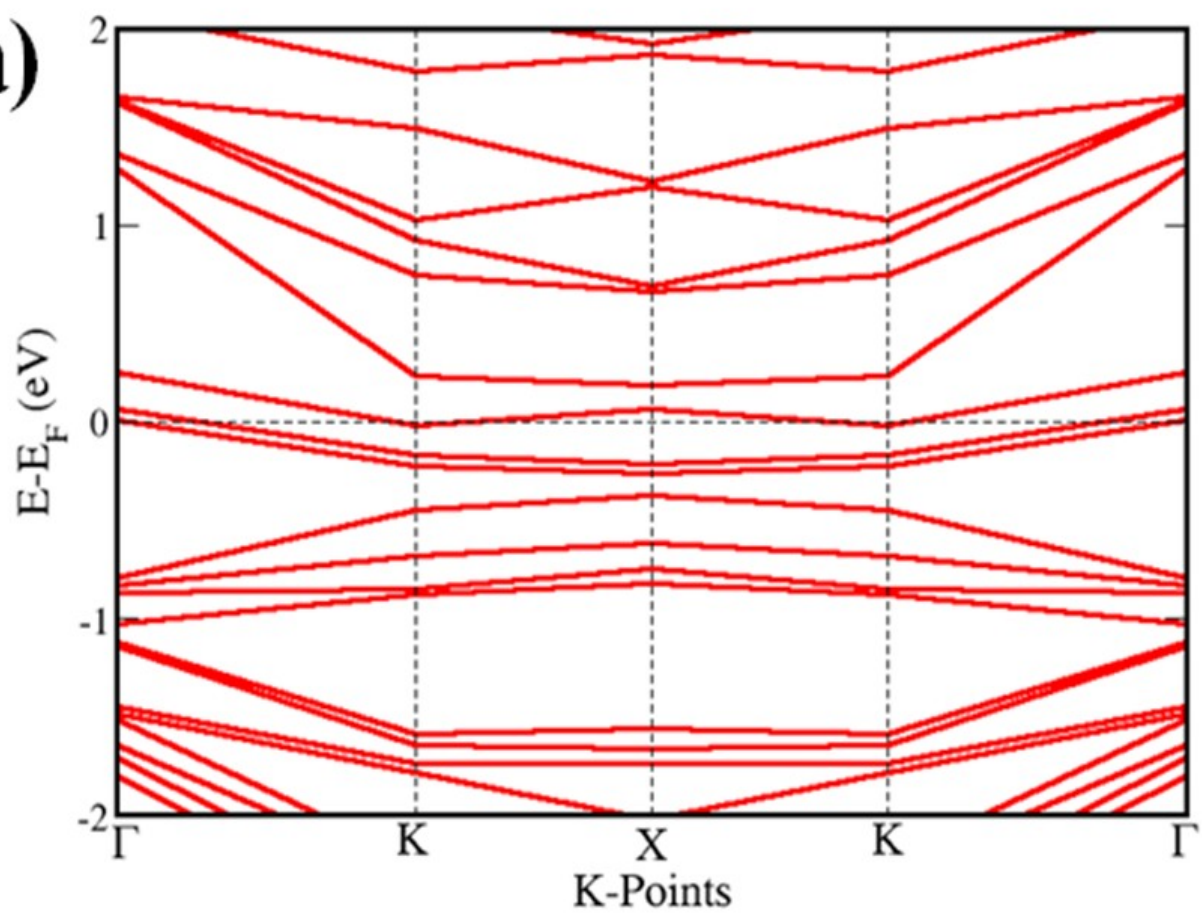
Supplementary Figure 3: Partial Density of States (PDOS) of O₂ gas molecule over MoB₂ Monolayer



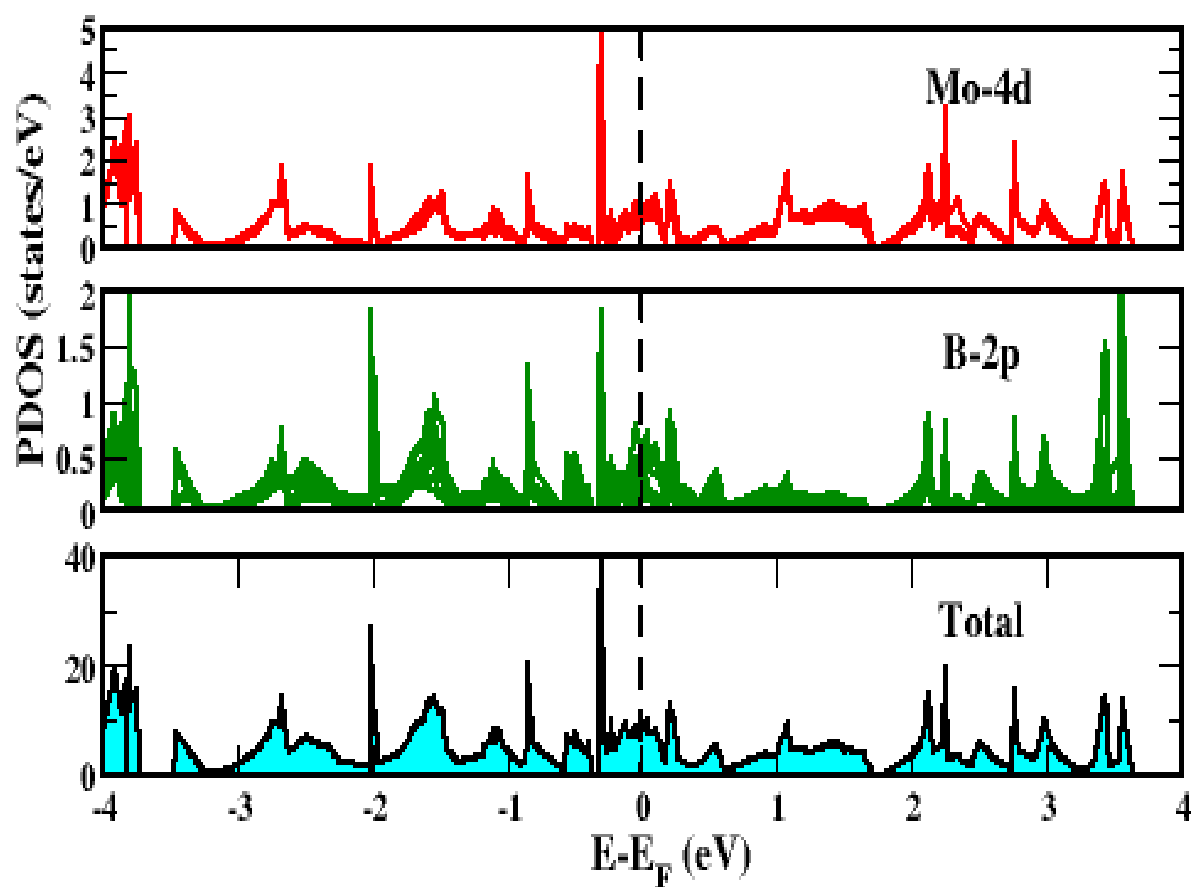
Supplementary Figure 4: Adsorption curve of O₂ adsorbed Monolayer showing physisorption nature.

Description: It can be seen from Figure 2(a) that there exists no interfacial bonding between the O₂ gas molecule and MoB₂ monolayer. This suggests that the nature of adsorption among the two species could be physisorption like in case of SO₂ adsorbed MoB₂ system. The charge sharing mechanism can also be seen from Figure 2(b) which confirms the presence of physisorption as there appears no electron flow between the MoB₂ monolayer and O₂ gas molecule. The existence of physisorption can also be justified by analysing the electronic structure of O₂ adsorbed MoB₂ monolayer. The partial density of states (PDOS) of the system is given in Figure 3 which clearly depicts that O-2p states are present in the valence band region and not participating in the metallic nature of the system. Only Mo-4d and B-2p states are actively participating in the metallic character of the material. In order to verify the physisorption nature we have also studied the adsorption curve given in Figure 4 which is following the similar trend like SO₂ adsorption curve (Fig 9 in main text). The minimum energy here is obtained at $d_{eq} \sim 2.0 \text{ \AA}$. Likewise SO₂ gas molecule, MoB₂ monolayer did not well detect the O₂ gas molecule. Hence we can claim that MoB₂ monolayer proves to be a good candidate for the sensing application particularly for NO₂ gas only.

a)



b)



Supplementary Figure 5: a) Energy Band, and b) Partial Density of States (PDOS) of pristine MoB₂ Monolayer