Supplementary Information

“An Ab-initio Study of Sensing Applications of MoB$_2$ Monolayer: A Potential Gas Sensor.”

Supplementary Figure 1: SO$_2$ gas molecule placed over MoB$_2$ monolayer showing a) S-up and b) S-down configuration.

Supplementary Figure 2: a) O$_2$ gas molecule placed over MoB$_2$ monolayer; [Note- Red double sided arrow indicates the interfacial distance $d_{eq} \approx 2.0\text{Å}$] and b) Charge dispersion schematics for O$_2$ gas molecule over MoB$_2$ monolayer.
Supplementary Figure 3: Partial Density of States (PDOS) of O$_2$ gas molecule over MoB$_2$ Monolayer
**Supplementary Figure 4:** Absorption curve of O$_2$ adsorbed Monolayer showing physisorption nature.

**Description:** It can be seen from Figure 2(a) that there exists no interfacial bonding between the O$_2$ gas molecule and MoB$_2$ monolayer. This suggests that the nature of adsorption among the two species could be physisorption like in case of SO$_2$ adsorbed MoB$_2$ 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 MoB$_2$ monolayer and O$_2$ gas molecule. The existence of physisorption can also be justified by analysing the electronic structure of O$_2$ adsorbed MoB$_2$ 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 valance 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 SO$_2$ adsorption curve (Fig 9 in main text). The minimum energy here is obtained at $d_{eq}$~2.0Å. Likewise SO$_2$ gas molecule, MoB$_2$ monolayer did not well detected the O$_2$ gas molecule. Hence we can claim that MoB$_2$ monolayer proves to be a good candidate for the sensing application particularly for NO$_2$ gas only.
Supplementary Figure 5: a) Energy Band, and b) Partial Density of States (PDOS) of pristine MoB$_2$ Monolayer