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# Supporting Information

## Realization of efficient and selective NO and $NO_2$ detection *via* surface functionalized h-$B_2S_2$ monolayer

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**Equation S1**: Calculation of binding energy ($E_b$). [1]

$$E_b = E_{Oh-B_2S_2} - E_{h-B_2S_2} - E_{atom}$$

$E_{Oh-B_2S_2}$, $E_{h-B_2S_2}$, and $E_{atom}$ indicates the total energy of oxygen functionalized h-$B_2S_2$, h-$B_2S_2$ and O-atom.

**Equation S2**: Calculation of cohesive energy ($E_{coh}$). [2]

$$E_{coh} = \frac{(2E_B + 2E_S + E_O) - E_{Oh-B_2S_2}}{5}$$

$E_B$, $E_S$, and $E_O$, are the energy of individual B-atom, S-atom, and O-atom, respectively. and $E_{Oh-B_2S_2}$ is the energy of the oxygen functionalized h-$B_2S_2$ monolayer.

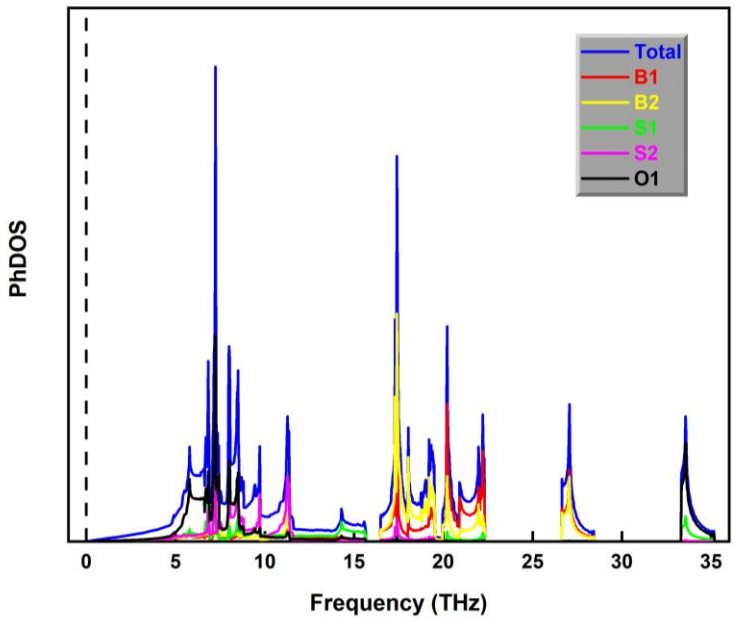



**Fig. S1**: Projected density of phonon states (PhDOS) plot of Oh-$B_2S_2$ monolayer.

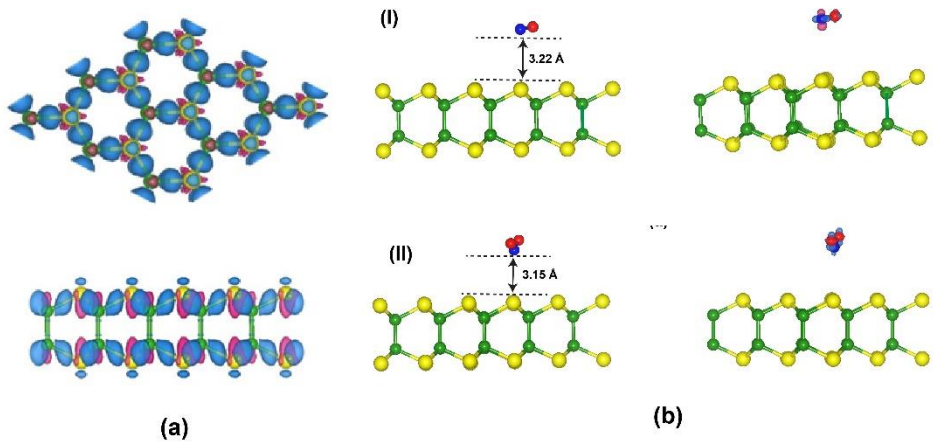



**Fig. S2:** (a) Charge density difference (CDD) plot of h-$B_2S_2$ monolayer (blue and pink colors indicate the charge accumulation and depletion region, respectively) and (b) most preferable adsorption configuration and CDD plots of (I) NO and (II) $NO_2$ adsorpbed h-$B_2S_2$ monolayer.

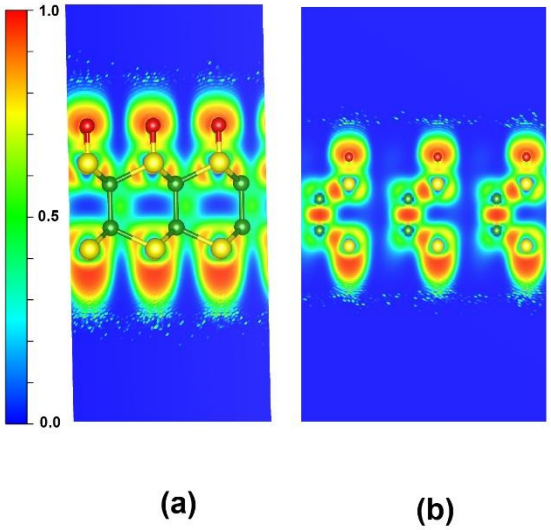
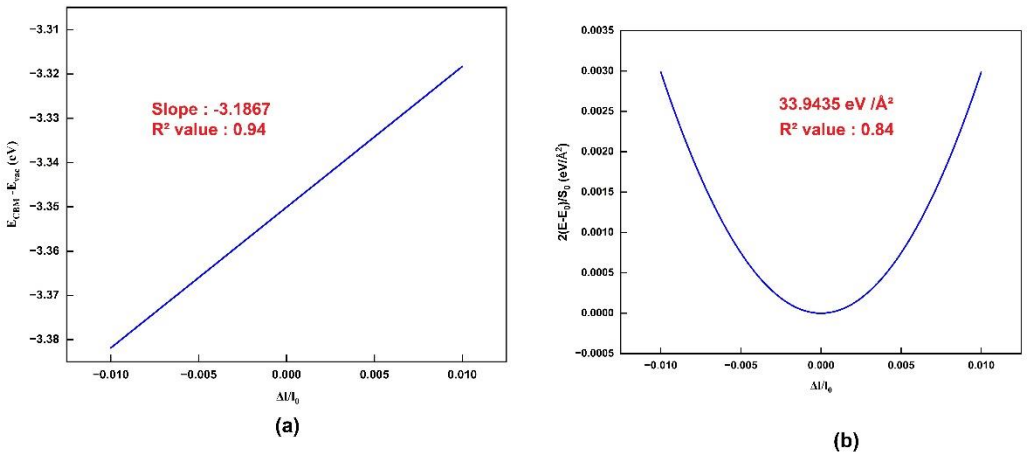



**Fig. S3**: Electron localization functions of oxygen functionalized h-$B_2S_2$ (Oh-$B_2S_2$) monolayer. ELF=1.0 (red color) indicates complete localization of electrons, while ELF=0.5 (green color) indicates delocalization. (a) 100-plane and (b) 110-plane.

**Table S1**: Binding energy ($E_b$) and S-O bond length of OT-$B_2S_2$ monolayer using PBE-GGA functional.

| Parameters | Calculated (Our results) | Reported (Previous work [1]) |
|---|---|---|
| Binding energy (eV) | -4.42 | -4.01 |
| S-O bond length (Å) | 1.47 | 1.48 |

**For h-$B_2S_2$ system**

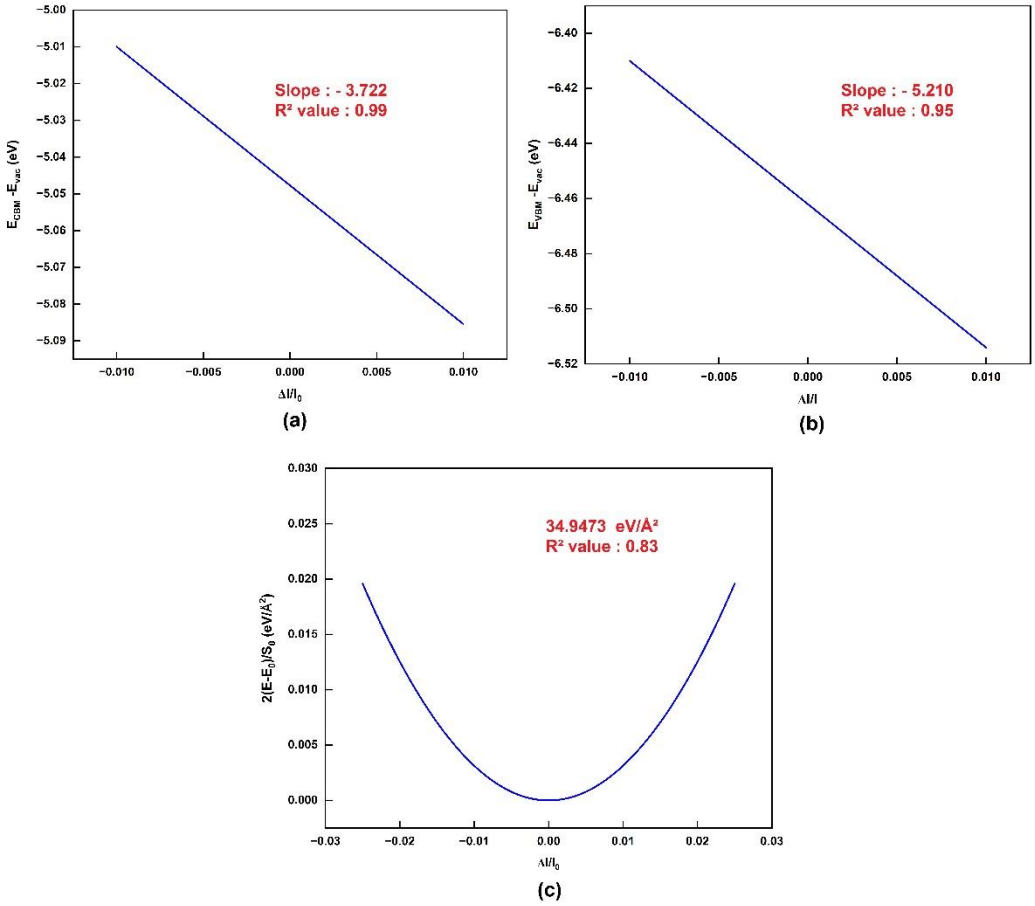



(a) Linear fitting of deformation potential and (b) curve fitting of elastic modulus of h-$B_2S_2$ monolayer.

**Calculated: μ (K-*Γ*): 1152.25 × $10^2$ $cm^2$ $V^{-1}$ $s^{-1}$**

**Reported [3]: μ (K-*Γ*): 1211.67 × $10^2$ $cm^2$ $V^{-1}$ s**

**For Oh-$B_2S_2$ system**

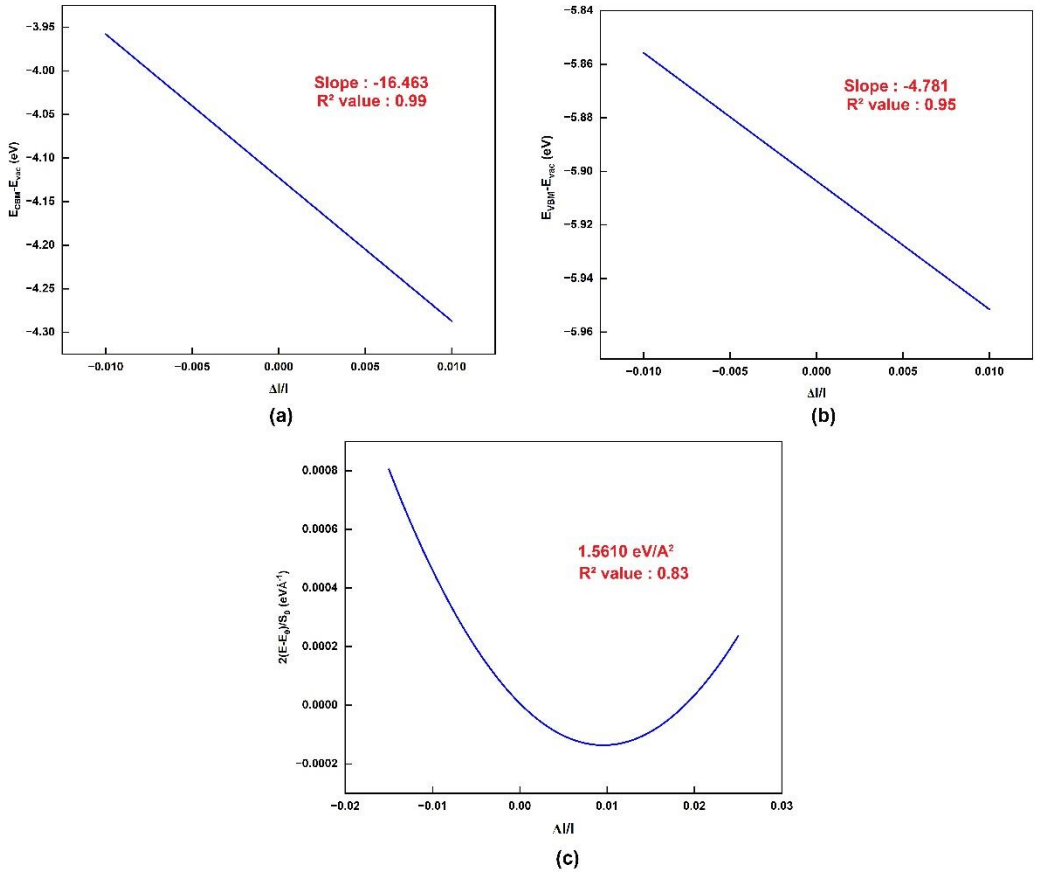



(a) Linear fitting of deformation potential for the electron, (b) Linear fitting of deformation potential for the hole, and (c) curve fitting of elastic modulus of Oh-$B_2S_2$ monolayer.

**Calculated: Electron mobility: μ (K-*Γ*): 790 × $10^2$ $cm^2$ $V^{-1}$ $s^{-1}$**

**Hole mobility: μ (K-*Γ*): 32 × $10^2$ $cm^2$ $V^{-1}$ $s^{-1}$**

**For $MoS_2$ system**




(a) Linear fitting of deformation potential for the electron, (b) Linear fitting of deformation potential for the hole, and (c) curve fitting of elastic modulus of $MoS_2$ monolayer.

**Calculated: Electron mobility: μ (K-M): 280 $cm^2 V^{-1} s^{-1}$**

**Hole mobility: μ (K-M): 161 $cm^2 V^{-1} s^{-1}$**

**Fig. S4:** Linear fitting deformation potential and curve fitting elastic modulus plots of h-$B_2S_2$, Oh-$B_2S_2$, and $MoS_2$.

**Table S2**: Effective mass and deformation potential of electrons and holes, and elastic modulus of $MoS_2$ and Oh-$B_2S_2$ monolayer.

| Systems | Effective mass ($M_0$) | | Deformation Potential | | Elastic Modulus ($J\ m^{-2}$) |
|---|---|---|---|---|---|
| | electron | hole | electron | hole | |
| $MoS_2$ | 0.45 (Reported) [4]<br>0.31 (Calculated) | 0.62 (Reported) [4]<br>0.43 (Calculated) | 16.46 | 4.78 | 246.60 |
| Oh-$B_2S_2$ | 0.11 | 0.31 | 3.72 | 5.2 | 559.15 |

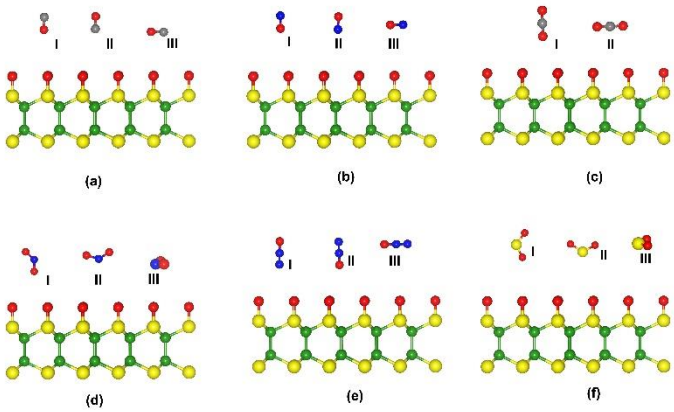



**Fig. S5:** Different orientations of (a) CO, (b) NO, (c) $CO_2$, (d) $NO_2$, (e) $N_2O$, and (f) $SO_2$ molecules on Oh-$B_2S_2$ monolayer.

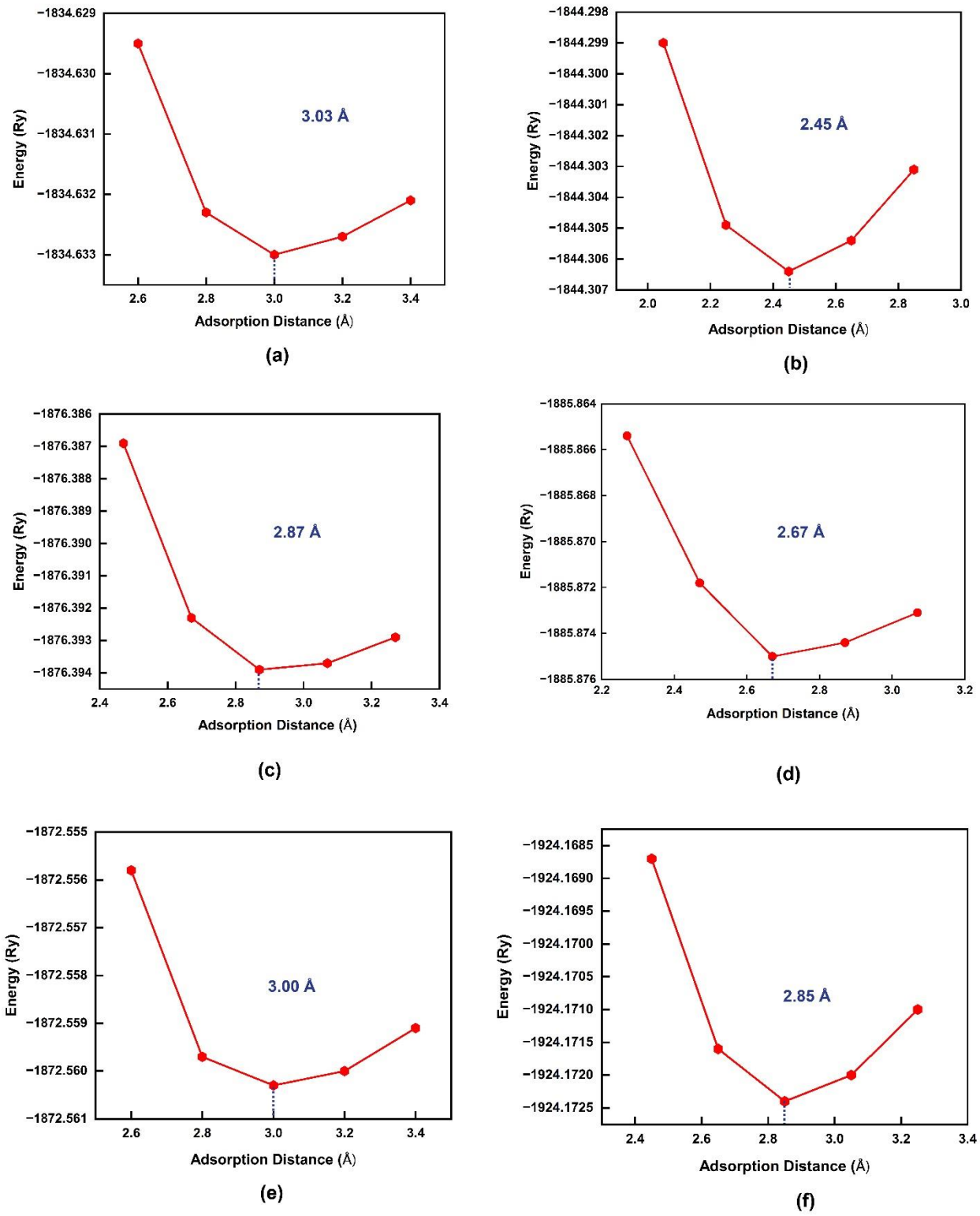



**Fig. S6**: Potential energy curves (PECs) of (a) CO, (b) NO, (c) $CO_2$, (d) $NO_2$, (e) $N_2O$, and (f) $SO_2$ molecules on Oh-$B_2S_2$ monolayer.

**Table S3**: Results obtained from spin-polarized density functional theory (SPDFT).

| Molecule/Supercell | $E_{ads}$ (eV) | AD (Å) | $Q_e$ |
|---|---|---|---|
| NO | -0.50 | 2.45 | 0.29 |
| $NO_2$ | -0.12 | 2.67 | 0.11 |

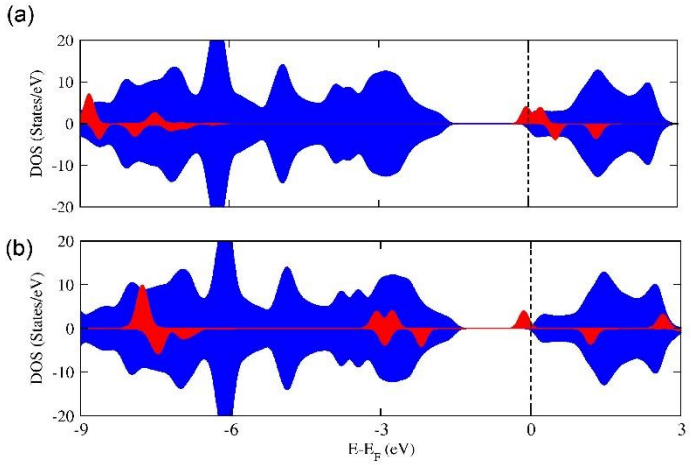



**Fig. S7**: Spin-polarized density of states (SPDOS) (a) NO and (b) $NO_2$ -adsorbed Oh-$B_2S_2$ monolayer. Blue and red are the density of states (DOS) of Oh-$B_2S_2$ monolayer and gas molecules, respectively.

**Table S4**: Adsorption energies ($E_{ads}$), adsorption distances (AD), and charge transfer ($Q_e$) values of NO and $NO_2$-adsorbed Oh-$B_2S_2$ monolayer for 4×4 and 5×5 supercells.

| Molecule/Supercell | $E_{ads}$ (eV) | AD (Å) | $Q_e$ |
|---|---|---|---|
| NO (3×3) | -0.56 | 2.45 | 0.34 |
| NO (4×4) | -0.57 | 2.45 | 0.34 |
| NO (5×5) | -0.60 | 2.46 | 0.33 |
| NO (3×3) | -0.16 | 2.65 | 0.13 |
| $NO_2$ (4×4) | -0.17 | 2.65 | 0.15 |
| $NO_2$ (5×5) | -0.17 | 2.67 | 0.14 |

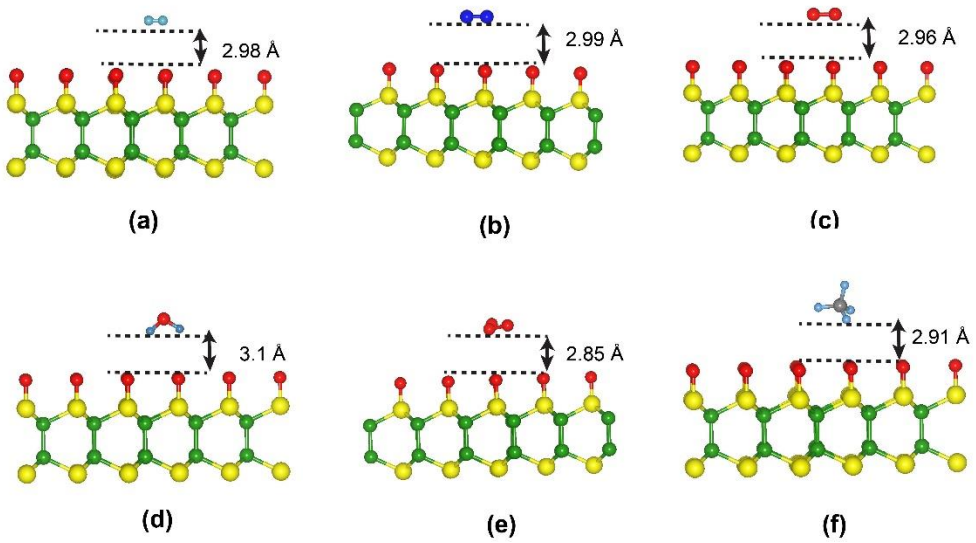



**Fig. S8**: The optimized geometries associated with the favorable adsorption configuration for (a) $H_2$, (b) $N_2$, (c) $O_2$ (d) $H_2O$, (e) $O_3$, and (f) $CH_4$ on Oh-$B_2S_2$ monolayer.

**Table S5**: Adsorption energies ($E_{ads}$) and charge transfer ($Q_e$) values of NO, $NO_2$, $H_2$, $N_2$, $O_2$, $H_2O$, $O_3$, and $CH_4$ on Oh-$B_2S_2$ monolayer.

| Gas Molecule | Orientation | $E_{ads}$ (eV) | $Q_e$ |
|---|---|---|---|
| NO | Parallel | -0.56 | 0.34 |
| | Through N | -0.50 | - |
| | Through O | -0.54 | - |
| $NO_2$ | Parallel | -0.16 | 0.13 |
| | Through N | -0.08 | - |
| | Through O | -0.15 | - |
| $H_2$ | Parallel | -0.03 | 0.004 |
| | Perpendicular | -0.03 | - |
| $N_2$ | Parallel | -0.07 | 0.007 |
| | Perpendicular | -0.05 | - |
| $O_2$ | Parallel | -0.09 | 0.08 |
| | Perpendicular | -0.07 | - |
| $H_2O$ | Parallel | -0.12 | 0.05 |
| | Through O | -0.11 | - |
| | Through H | -0.08 | - |
| $O_3$ | Parallel | -0.10 | 0.02 |
| | Perpendicular | -0.06 | - |
| $CH_4$ | Parallel | -0.10 | 0.02 |
| | Perpendicular | -0.10 | - |

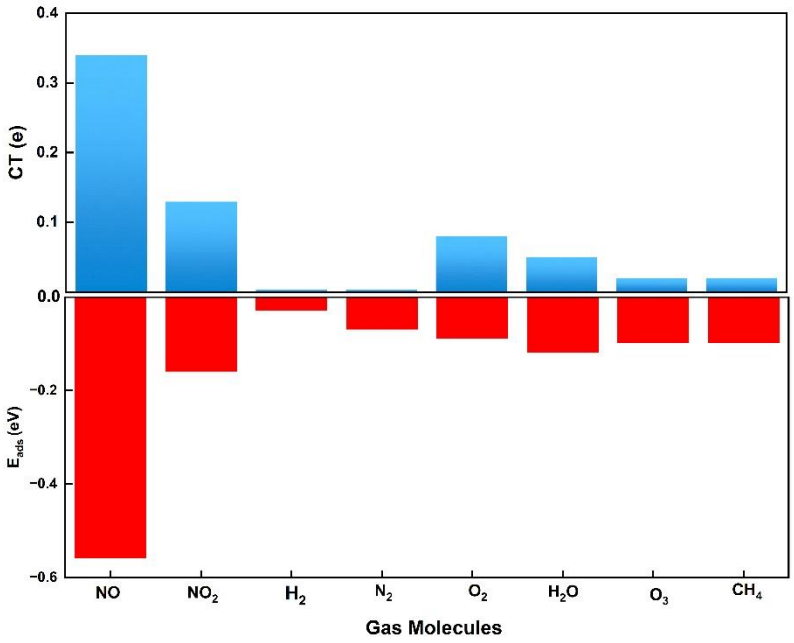



**Fig. S9**: Adsorption energies ($E_{ads}$) and charge transfer ($Q_e$) plots of NO, $NO_2$, $H_2$, $N_2$, $O_2$, $H_2O$, $O_3$, and $CH_4$ on Oh-$B_2S_2$ monolayer.

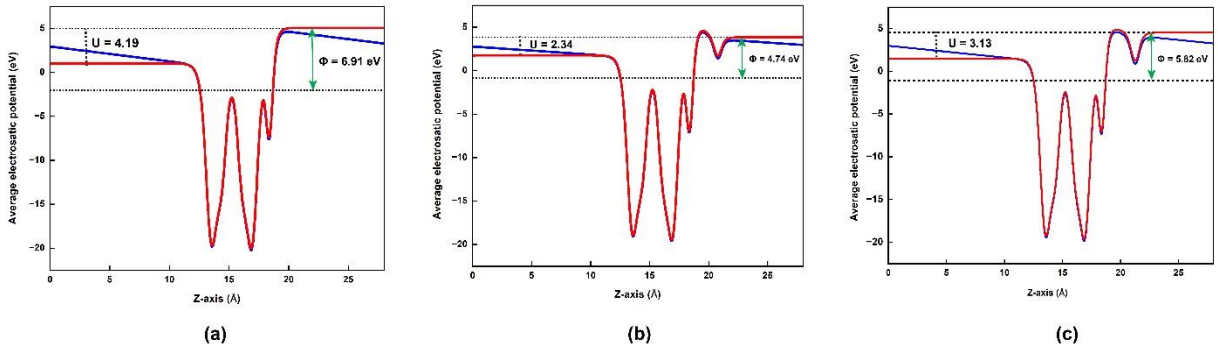



**Fig. S10**: Average electrostatic potential plots of (a) Oh-$B_2S_2$, (b) NO-adsorbed Oh-$B_2S_2$, and (c) $NO_2$-adsorbed Oh-$B_2S_2$ monolayer. The blue and red plots depict the without dipole correction and with dipole correction.

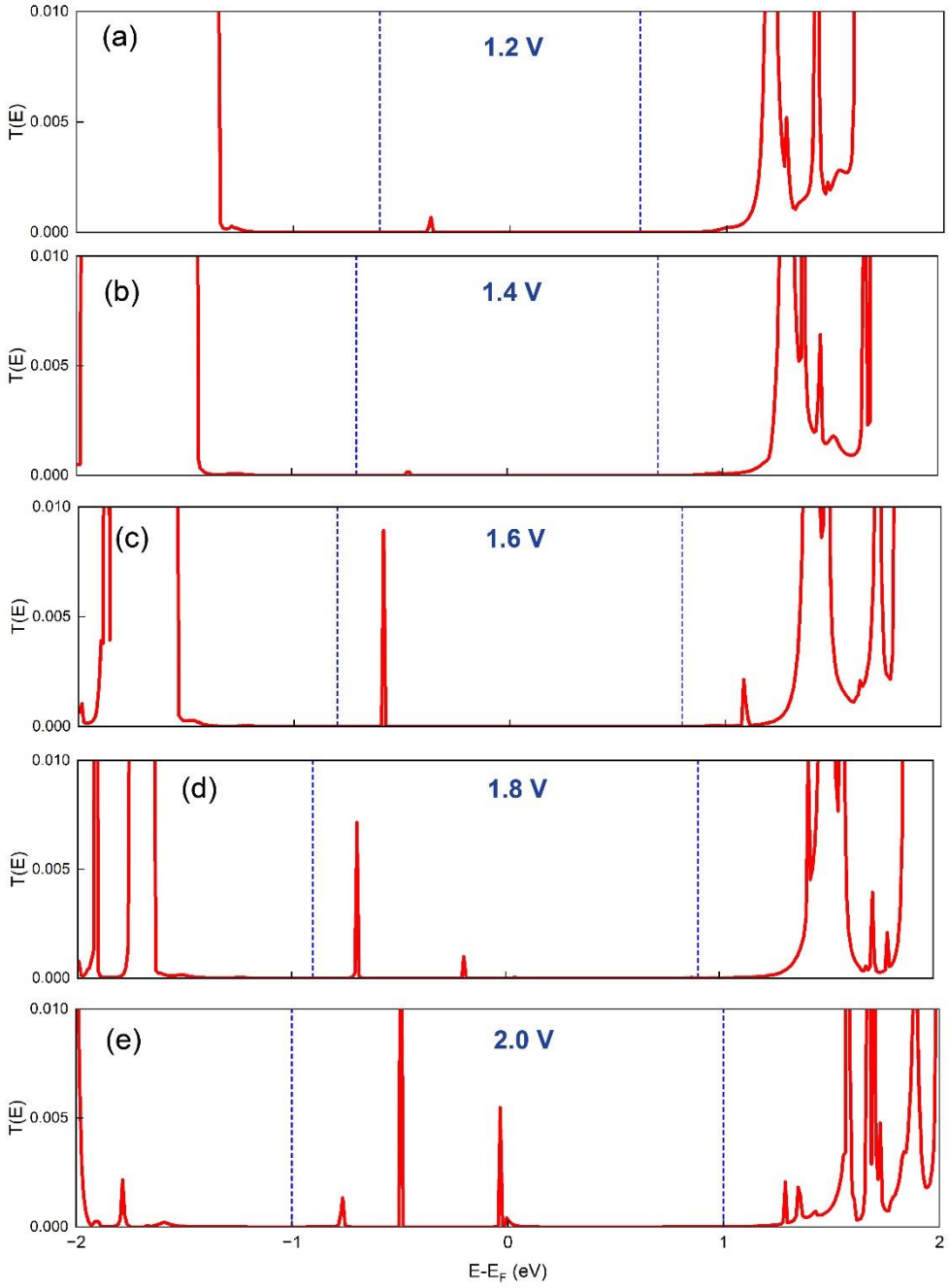



**Fig. S11**: Transmission spectra T(E) plots of Oh-$B_2S_2$ at different bias voltages.

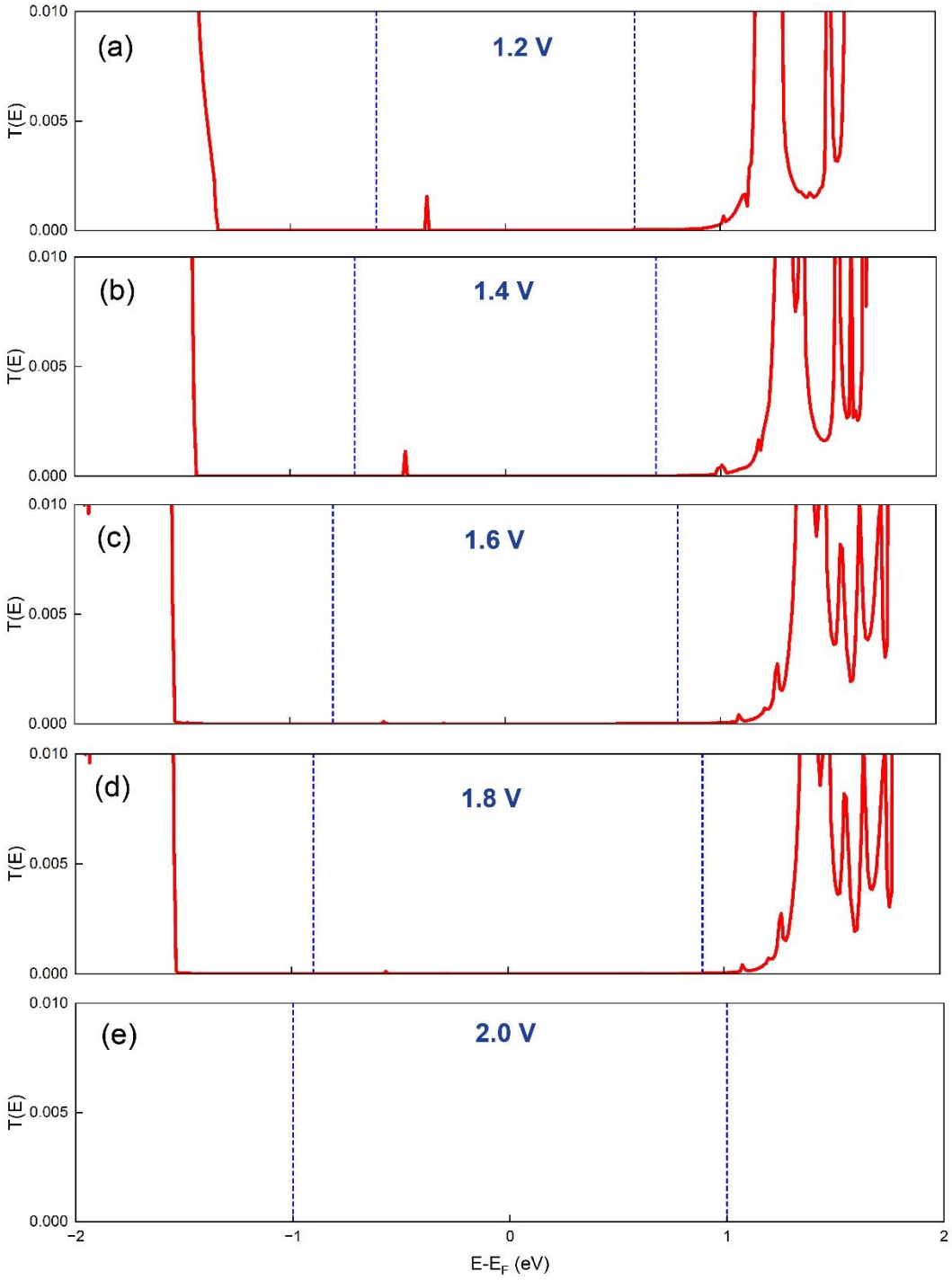



**Fig. S12**: Transmission spectra T(E) plots of NO-adsorbed Oh-$B_2S_2$ at different bias voltages.

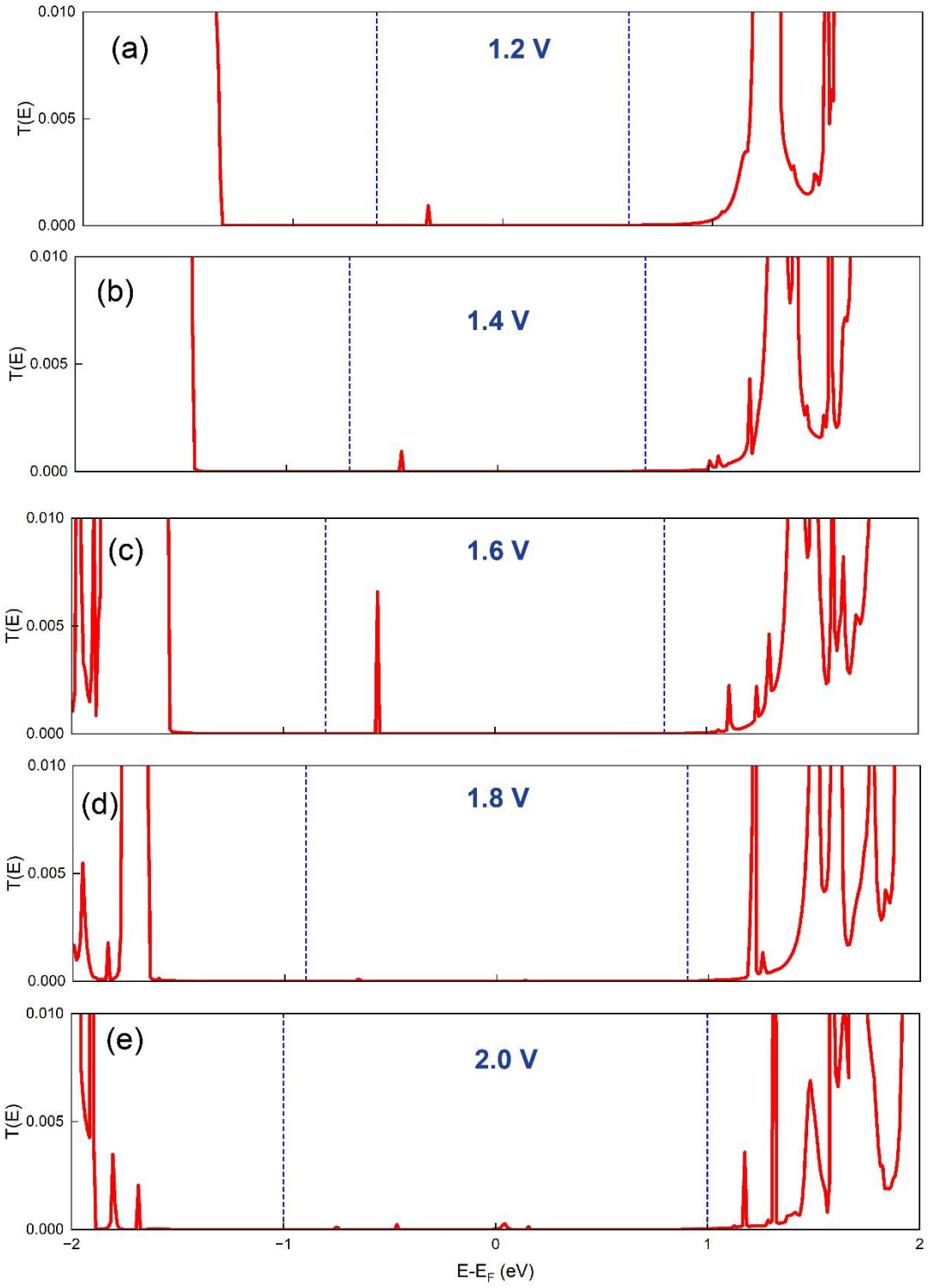



**Fig. S13**: Transmission spectra T(E) plots of $NO_2$-adsorbed Oh-$B_2S_2$ at different bias voltages.

## References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