

Simulation of Two-Dimensional MoS₂ for Gas Sensing Applications

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Outline

- **Backgrounds and Motivation**
- **Computational Methods**
- **Results and Discussion**
- **Conclusions**

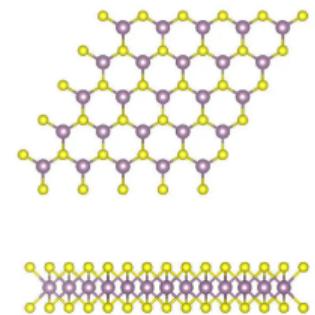
Background & Motivation

- ▶ The growing demand for detecting toxic gases requires highly sensitive, low-noise, and energy-efficient gas sensors.
- ▶ Monolayer MoS₂ is a promising sensing material due to its direct band gap (~1.9 eV) and high surface-to-volume ratio, which enhance its sensitivity to gas adsorption.
- ▶ First-principles DFT simulations provide fundamental insight into adsorption energy, charge transfer, and electronic structure changes of MoS₂ upon gas adsorption.

source : Yue *et al.*, *Nanoscale Res. Lett.* **8**, 425 (2013).

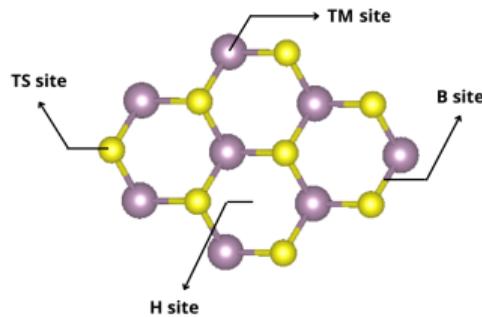
Computational Method

- ▶ DFT calculations using QUANTUM ESPRESSO with PAW pseudopotentials, and VESTA / XCrySDen for visualization.
- ▶ Spin-polarized calculations for open-shell gas molecules.
- ▶ Plane-wave cutoff energy: 30 Ry.
- ▶ $5 \times 5 \times 1$ ($10 \times 10 \times 1$ for DOS) Monkhorst–Pack k -point mesh.
- ▶ 4×4 monolayer MoS₂ supercell with 20 Å vacuum spacing.
- ▶ Lattice constant was set to 3.12 Å, supercell 4x4 = 12.48 Å.



Configuration of the single-layer MoS₂ computational model

Computational Method



Simulation Parameters

- ▶ **Molecular Target:**
 H_2, O_2, H_2O, NO, NO_2 , dan CO .
- ▶ **Adsorption Position:**
On-top on the site: T_M (Top-Mo), T_S (Top-S), H (Hollow), dan B (Bridge).
- ▶ **Initial Orientation:**
 Position Variations **Vertical & Horizontal** (find minimum energy).
- ▶ **Adsorption Energy (E_{ads}):**

$$E_{ads} = E_{tot} - (E_{MoS_2} + E_{gas})$$

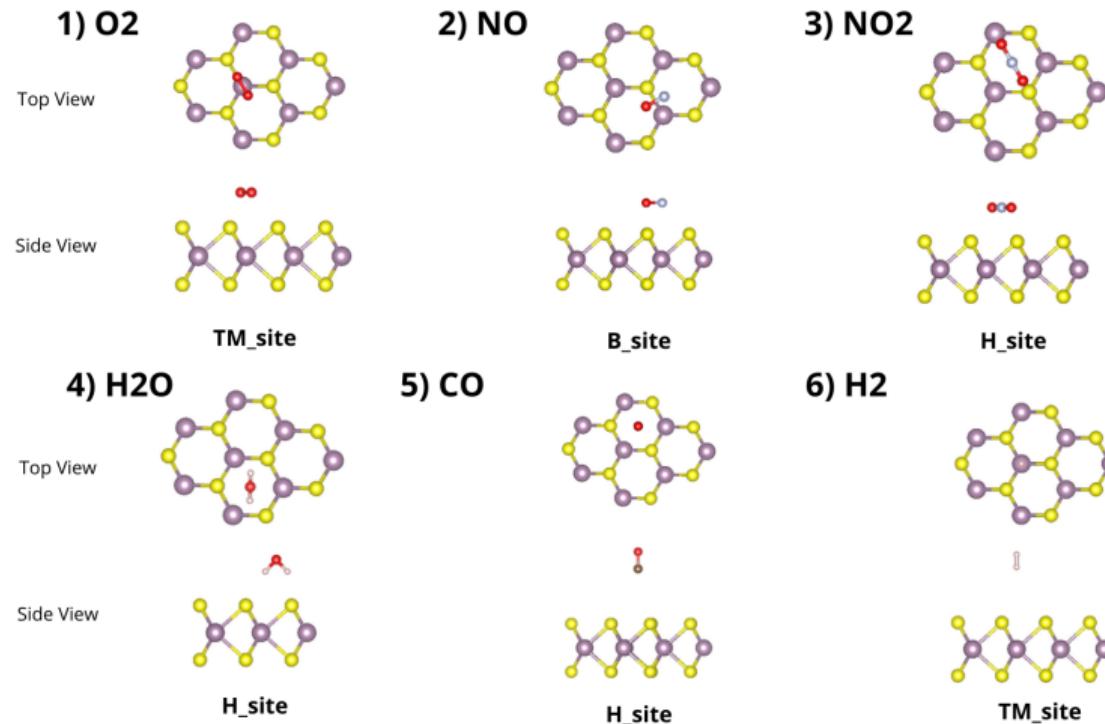
Negative = Stable / Exothermic

Results for Gas Molecules on Monolayer MoS₂

Gas	H site E_a (meV)	TM site E_a (meV)	TS site E_a (meV)	B site E_a (meV)
H ₂	-40.9013	-43.7774	-5.8134	-41.8101
O ₂	1092.8685	-67.6157	2080.8573	218.3902
NO	-85.5102	-90.6396	-86.9116	-91.9581
NO ₂	-1584.2736	-1577.4380	-1554.1416	—
CO	-266.9261	—	—	—
H ₂ O	-115.7200	-107.4448	-103.3233	-112.9846

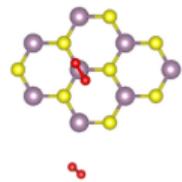
E_a was calculated as $E_a = E_{\text{MoS}_2+\text{gas}} - (E_{\text{MoS}_2} + E_{\text{gas}})$. Negative values indicate exothermic adsorption.

Adsorption Configurations on Monolayer MoS₂

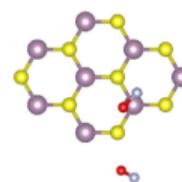


Relaxed Atomic Configuration

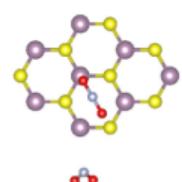
1) O₂



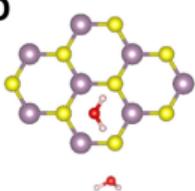
2) NO



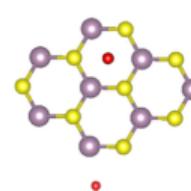
3) NO₂



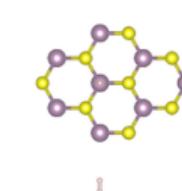
3) H₂O



3) CO



3) H₂

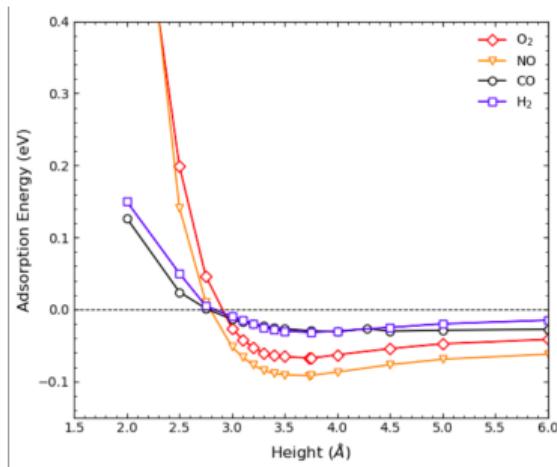


Adsorption Energy of Gas Molecules on Monolayer MoS₂

Gas	Site	h (Å)	E_a (meV)
H ₂	TM	3.74	-43.78
O ₂	TM	3.72	-67.62
NO	B	3.72	-91.95
NO ₂	H	3.50	-1577.44
H ₂ O	H	3.44	-115.72
CO	H	4.23	-26.69

- ▶ **NO₂**: Largest adsorption energy, indicating strong chemisorption.
- ▶ **H₂O and NO**: Moderate adsorption energies, suggesting stable interactions.
- ▶ **H₂ and CO**: Very small adsorption energies, indicating weak interactions.

Adsorption Height Variation



High Equilibrium Calculation

$$H_{eq} = \frac{\sum (z_i \cdot m_i)}{M_{total}} - z_{S,max}$$

z_i is vertical coordinate for atom molecule.

Adsorption Analysis:

Methodology:

H_{eq} was varied (2–6 Å) based on the molecule's CoM to find E_{min} .

Adsorption Strength:

NO shows the strongest binding energy; H_2 is the weakest.

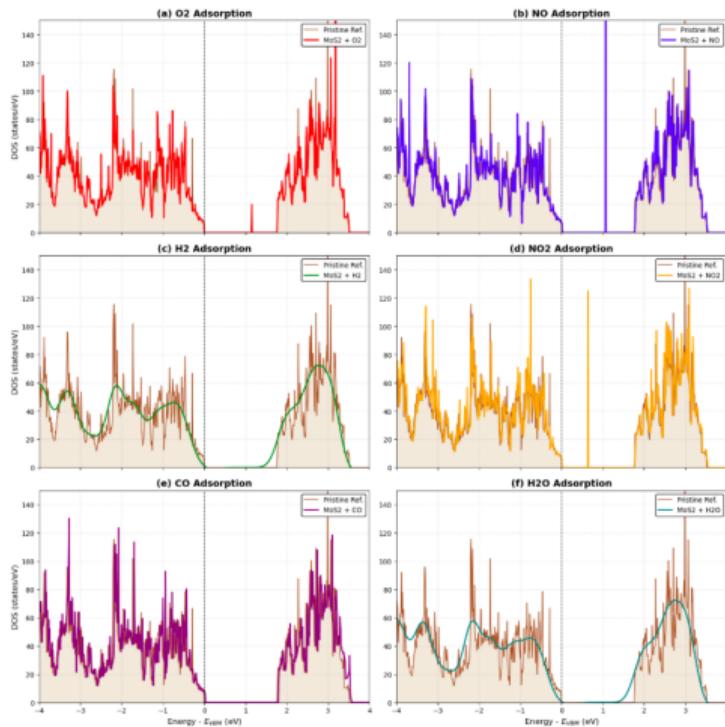
Asymptotic Limit:

Energy approaches zero at $h \approx 5.0$ Å, marking the limit of interaction.

Physisorption:

Confirmed by low E_a and large equilibrium distance (H_{eq}).

Density of States Analysis

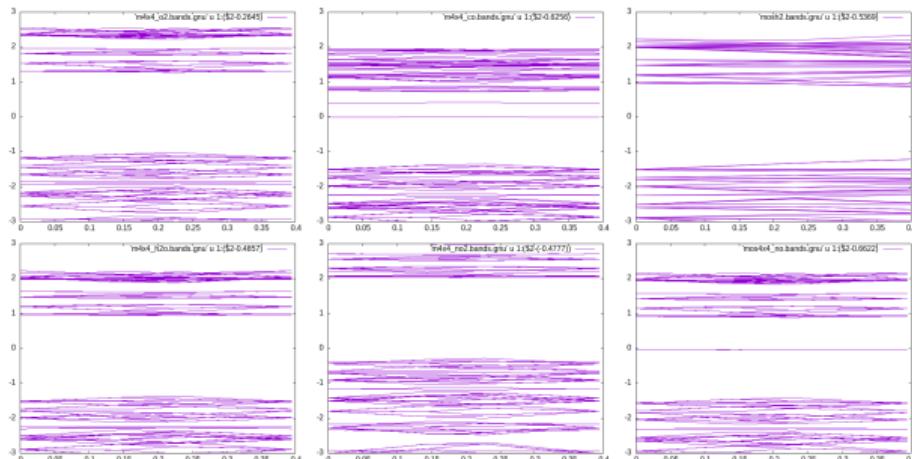


DOS Plots: (a) O_2 , (b) NO , (c) H_2 , (d) NO_2 , (e) CO , (f) H_2O .

Key Observations:

- ▶ Main peaks and band gap (~ 1.78 eV) remain largely unchanged, verifying weak physical adsorption.
- ▶ Impurity States & Sensing (O_2, NO, NO_2): Sharp spikes within the gap act as electron traps or bridges.
- ▶ Stable Profiles (H_2, H_2O): Smooth, non-magnetic curves without gap spikes reflect high electronic stability.

Band Structure of Gas-Adsorbed Monolayer MoS₂



Band structures referenced to the Fermi level for different gas molecules.

- ▶ Weak adsorption (H₂, CO): minimal electronic perturbation.
- ▶ Strong adsorption (NO, NO₂): impurity states and band gap narrowing.
- ▶ Band modulation governs the gas sensing response of MoS₂.

Conclusions

- ▶ **Adsorption Mechanism (Physisorption):**

Calculated energies confirm weak interaction (physisorption). This suggests the sensor allows for easy *desorption* (reset process) and reusability.

- ▶ **Electronic Selectivity:**

While the primary band gap remains stable (mimicking pristine MoS_2), gases (NO_2 , O_2 , NO) induce unique **impurity states** in the gap, proving the material's ability to distinguish gas types.

- ▶ **Charge Transfer Evidence:**

DOS and Band Structure analyses confirm the presence of charge transfer (gases acting as acceptors/donors), although specific quantitative values (Bader charge) are reserved for future work.

- ▶ **Sensor Viability:**

The study confirms monolayer MoS_2 as a promising candidate for **FET-based gas sensors**, offering distinct electronic signatures for detection with high energy efficiency.

THE MICROSCOPIC ADVENTURES OF 2D MoS₂ & THE GAS GANG! (A Simulation Story)

THE CHALLENGE: SNEAKY GASES



Gases are masters of disguise.
We need a material detective!

RESULTS: SENSITIVITY SMACKDOWN



MoS₂ shows a *shocking* change in resistance!
(It's super effective!)

THE SIMULATION SPELLBOOK (DFT)

Kohn-Sham equation

$$E[n] = T_s[n] + \int V_{\text{ext}}(\mathbf{r})n(\mathbf{r})d\mathbf{r} + E_H[n] + E_{\text{xc}}[n]$$

BEHOLD!
The Density Functional Theory!
(Don't try solving this by hand, mortals!)

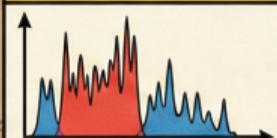
$$\frac{\partial^2 \sigma_{\text{ext}}}{\partial n^2} + (\hat{O} + \hat{o})$$

BAND GAP ROLLERCOASTER



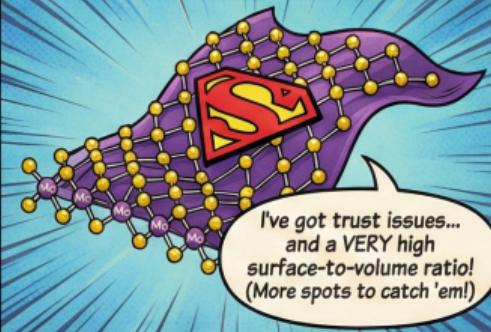
Direct Band Gap (~1.8 eV)! Wheee!
(No layovers for electrons!)

DENSITY OF STATES PARTY



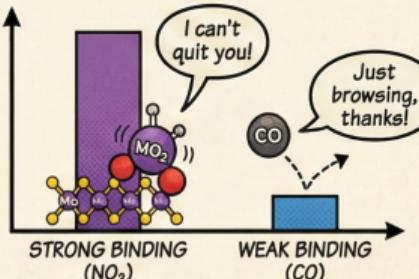
Valence Band: It's getting crowded in here!

THE HERO MATERIAL: 2D MoS₂ CAPE



I've got trust issues...
and a VERY high
surface-to-volume ratio!
(More spots to catch 'em!)

ADSORPTION ENERGY: STICKY SITUATIONS



Some gases stick like a bad nickname,
others just ghost us!

CONCLUSION & FUTURE MISSION: MoS₂ is a promising gas sensor sidekick! Next up: Experimental validation (and more coffee for the scientists)! TO BE CONTINUED...

Hatur Nuhun

Terima kasih atas perhatian Anda