Simulation of Two-Dimensional MoS_2 for Gas Sensing Applications

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Outline

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

Background & Motivation

- **Gas Sensing Challenge**
  Toxic gases such as CO, NO_2, and NO, as well as reactive and environmentally relevant gases (O_2, H_2, CO_2), require sensitive and low-power gas sensors.
- **Why Monolayer MoS_2**
  A direct band gap (~1.9 eV) and high surface-to-volume ratio make monolayer MoS_2 highly responsive to gas adsorption.
- **Why First-Principles Simulation**
  DFT provides insight into adsorption energy, charge transfer, and electronic response of MoS_2.

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 MoS_2 supercell with 20 Å vacuum spacing.

Configuration of the single-layer MoS_2 computational model

Computational Method

Simulation Parameters

- **Molecular Target:**
  H_2, O_2, H_2O, NO, NO_2, dan CO.
- **Adsorption Position:**
  On-top pada situs: 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 MoS_2 (GGA-PBE)

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	4158.4510
CO	-266.9261	–	–	–
H_2O	-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 MoS_2

Relaxed Atomic Configuration

1) O2

2) NO

3) NO2

3) H2O

3) CO

3) H2

Adsorption Energy of Gas Molecules on Monolayer MoS_2

Gas	Site	h (Å)	E_a (meV)
H_2	TM	3.50	-42.85
O_2	TM	3.75	-67.65
NO	B	3.72	-91.95
NO_2	H	3.50	-1577.44
H_2O	H	3.44	-115.72
CO	H	4.00	-31.19

Adsorption Height Variation

Key Insights:

- **Equilibrium:**

  Lowest point marks the stable position (E_{min} at h_{eq}).

- **Weak Interaction:**

  Flat curves near 0 imply weak van der Waals forces at $h \approx 3.0 - 3.2$ Å.

- **Physisorption:**

  Low energy (< 0.5 eV) and large separation (> 3.0 Å) confirm physical adsorption.

Density of States Analysis

Key Observations:

- **Intact Band Gap (≈ 1.78 eV):** Electronic structure preserved across all cases. Confirms *physisorption* without structural damage.
- **Impurity States (NO, NO_2, O_2):** Sharp mid-gap peaks emerge. Acts as bridges for charge transfer.
- **H_2 & H_2O Profile:** Smooth curves due to *Gaussian Smearing* parameters. Indicates minimal electronic perturbation.

Band Structure of Gas-Adsorbed Monolayer MoS_2

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

- Weak adsorption (H_2, CO): minimal electronic perturbation.
- Strong adsorption (NO, NO_2): impurity states and band gap narrowing.
- Band modulation governs the gas sensing response of MoS_2.

Summary

- **Visuals:** Flexible Grid Layouts.

Thank You!

Any Questions?

THE MICROSCOPIC ADVENTURES OF 2D MoS_2 & THE GAS GANG! (A Simulation Story)

THE CHALLENGE: SNEAKY GASES

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

THE SIMULATION SPELLBOOK (DFT)

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 MoS_2 CAPE

RESULTS: SENSITIVITY SMACKDOWN

MoS_2 shows a *shocking* change in resistance!
(It's super effective!)

ADSORPTION ENERGY: STICKY SITUATIONS

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

CONCLUSION & FUTURE MISSION: MoS_2 is a promising gas sensor sidekick! Next up: Experimental validation (and more coffee for the scientists)! TO BE CONTINUED...