A First principles study on gas sensing properties of novel 2D In_2O_3 layer

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Two-dimensional (2D) materials have garnered significant attention for gas sensing applications due to their exceptional properties, including a high surface-to-volume ratio, excellent electrical conductivity, tunable electronic structure, mechanical flexibility, and the potential for functionalization to improve sensitivity and selectivity. In this study, we employ first-principles calculations to explore the gas-sensing performance of a recently proposed In_2O_3 monolayer [1]. Specifically, we evaluate its interaction with six harmful gases—CO_2, SO_2, NO_2, H_2S, NO, and NH_3—as well as its response to common ambient molecules (CO_2, O_2, and H_2O) to assess its viability in real-world sensing environments.
Our findings reveal that the In_2O_3 monolayer exhibits optimal adsorption energy and a significant resistance change upon NO adsorption, underscoring its excellent sensitivity and selectivity for NO detection. While NH_3 and H_2S show slightly enhanced adsorption energy, they do not induce a notable resistance change, indicating limited sensing capability for these gases. Regarding ambient molecules, O_2 and CO_2 display weak adsorption, minimizing interference, whereas H_2O exhibits moderate adsorption, which could hinder sensor performance in humid conditions.
Overall, our study establishes the In_2O_3 monolayer as a promising candidate for next-generation 2D gas sensors, particularly for highly selective and sensitive NO detection.

References

[1] Ruishen Meng, et. al., J. Appl. Phys. 128, 034304 (2020).

Figures

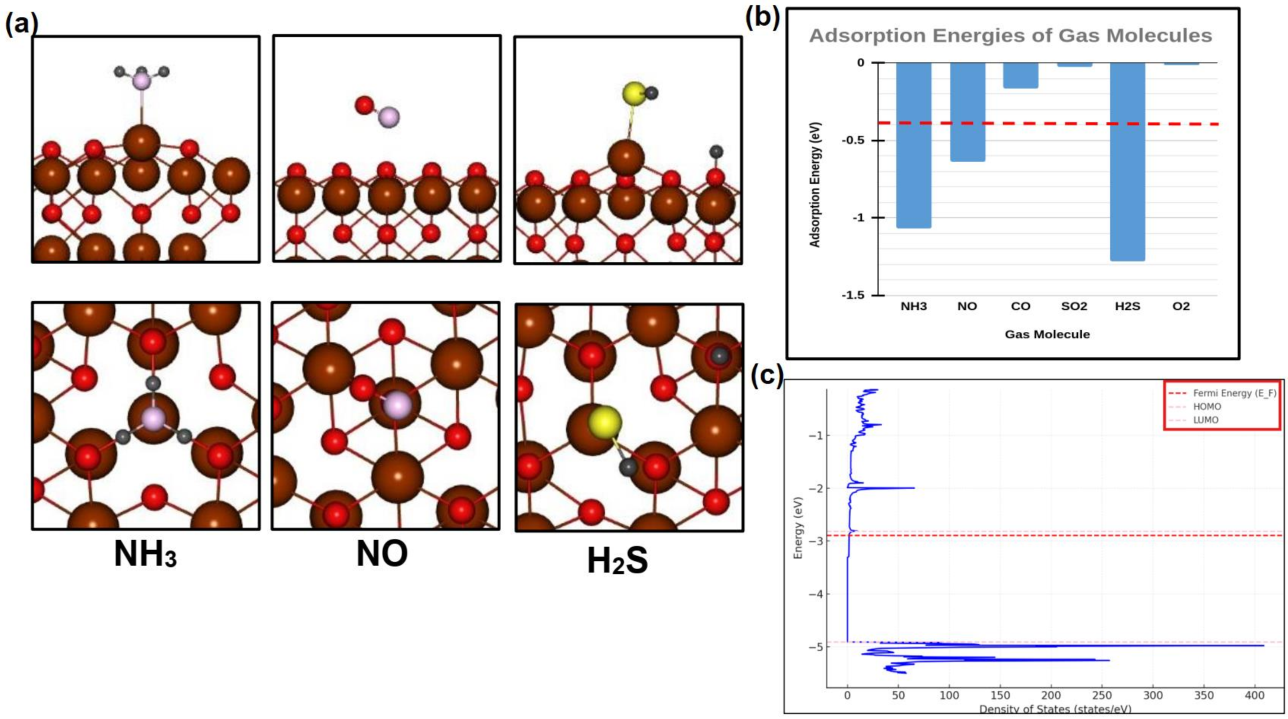

Figure 1: (a) Adsorption configuration of the harmful gas molecules that display suitable adsorption energy, namely NH_3, NO and H_2S. Top panel: side view, Bottom panel: top view (b) Adsorption energy of different gas molecules, under investigation, on the surface of In_2O_3 monolayer (c) Density of states of NO adsorbed In_2O_3 monolayer, demonstrating the Fermi energy have penetrated inside the conduction band resulting in a large change in conductivity.