

Self-Powered Gas Sensing in Interface Engineered 2D layered Heterostructures

Dipanjana Mondal¹, Vinayak Kamble^{1,*}

¹*School of Physics, Indian Institute of Science Education and Research Thiruvananthapuram, Kerala, India 695551.*

**email: kbvinayak@iisertvm.ac.in*

Summary:

The development of self-powered gas sensors is critical for enabling low-power, autonomous sensing systems, yet achieving high sensing performance without external bias remains a significant challenge. Self-powered gas sensing, enabled by built-in electric fields at carefully engineered heterointerfaces, offers a compelling pathway beyond this limitation. In this work, we present a comparative investigation of self-powered gas sensors based on both Transition metal dichalcogenide (TMD)-oxide and TMD-TMD interfaces. The three distinct 2D interface devices studied here are, MoSe₂-MoO₂, MoS₂-MoO₂ and ReS₂-MoS₂, employed via single-step CVD method. Across all three systems, reproducible zero-bias sensing responses and enhanced performance under photo-activation are observed, pointing to interface-driven charge separation as the governing mechanism. These findings collectively establish a generalized design framework in which interface engineering underpins self-powered sensing behaviour, rather than material choice alone.

Keywords: Self-powered gas Sensor, 2D materials, heterostructure, Transition Metal Dichalcogenides, Interface engineering

Background, Motivation and Objective

The growing demand for continuous environmental and health monitoring has intensified the need for gas sensors that operate reliably without a power supply. Conventional chemiresistive and metal-oxide based sensors typically require elevated operating temperatures (100-400 °C)¹ or continuous external biasing to achieve adequate sensitivity, making them ill-suited for battery-constrained wearables, and remote Internet-of-Things nodes. 2D TMDs have emerged as a promising platform to address this challenge, owing to their atomically thin geometry, large surface-to-volume ration, tunable bandgap, and strong light-matter coupling. Recent studies have demonstrated that heterostructure formation can induce built-in electric fields, enabling spontaneous charge separation and self-powered operation².

Despite rapid progress in individual TMD-based sensors, a systematic understanding of interface behaviour governs self-powered sensing performance remains lacking. Most existing studies focus on individual material systems, limiting the ability to derive general design principles. In particular, the interplay between band alignment, defect states, and photo-induced carrier

dynamics across diverse heterostructure is not yet fully understood³.

In this work, we aim to bridge this gap by investigating multiple CVD-grown 2D heterostructures and identifying common physical mechanisms governing self-powered gas sensing⁴. The objective is to move beyond material-specific observations and establish a generalized framework based on interface-driven charge dynamics applicable to next-generation autonomous sensors.

Description of the New Method or System

Here, we have studied three heterostructure systems synthesized by single-step CVD method to ensure clean, scalable, defect free interface formation without intermediate transfer-related contamination. Comprehensive structural and spectroscopic characterization like Raman, PL, XPS, HR-TEM are performed to confirm the integrity of the interface and the compositional gradation within individual flakes.

The first system, MoSe₂-MoO₂ heterostructure is a single flake metal-semiconductor heterointerface. Due to heterostructure formation, band-alignment establishes a built-in electric field capable of driving photoinduced carrier separation without external bias. The second system

introduces MoS₂-MoO₂ as a structurally analogous yet chemically distinct TMD-oxide platform⁵. The distinct sulphur-based chemistry relative to the selenide system modifies the charge redistribution at the interface. Thus, this provides a direct opportunity to isolate the role of chalcogen identity on the self-powered sensing response, independent of geometric or structural differences. Finally, the third system, ReS₂-MoS₂, represents a fundamentally different class of interface, i.e., a TMD-TMD van der Waals junction. This heterostructure generates a type-II staggered band alignment, which promotes spatial separation of photoexcited carriers across the junction, enabling self-powered current transduction upon gas exposure.

Results

All investigated heterostructure exhibit measurable gas sensing response towards NO₂ gas under zero external bias as shown in the insets of Figure 1, confirming their self-powered operation. Under illumination, a pronounced enhancement in sensing behaviour is observed across all systems (Figure 1). This photo-induced response indicates that light plays a significant role in facilitating carrier generation and improving charge separation efficiency. Furthermore, the extent of enhancement varies among heterostructures, suggesting that the coupling between optical absorption and interfacial charge transfer is system-dependent. Thus, the cross-system comparative analysis reveals that the built-in electric field at the 2D heterointerface is sufficient to drive measurable zero-bias sensing. Additionally, the enhancement under illumination suggests photoinduced carrier separation as demonstrated in the schematic in Figure 1 (right panel). The relative contribution of each factor depends on the specific heterostructure, but the underlying principle remains consistent across all systems. Therefore, this highlights the importance of interface engineering as a primary design strategy for self-powered sensing devices.

Conclusion

In summary, we demonstrated a comparative study of multiple 2D heterostructure to establish a generalized understanding of self-powered gas sensing. By examining both TMD-oxide and TMD-TMD interfaces, we demonstrate that interface-driven charge dynamics and photo-assisted processes govern sensor performance. The findings move beyond material specific observations and provide a unified framework for designing next-generation self-powered gas sensors.

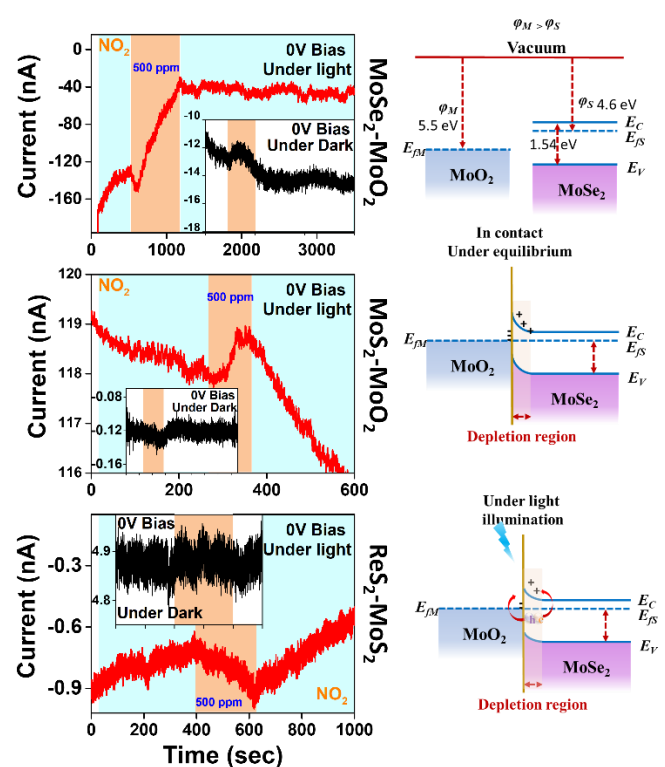


Fig. 1. (left column) The response to NO₂ gas (500 ppm) at room temperature under dark and under light illumination for (top to bottom) MoSe₂-MoO₂, MoS₂-MoO₂ and ReS₂-MoS₂ heterostructure flakes. (right column) the band diagram under flat band condition, with heterostructure formation and under light illumination.

References

- [1] Barsan, N.; Weimar, U., Conduction model of metal oxide gas sensors. *Journal of Electroceramics* **2001**, 7 (3), 143-167.
- [2] Qiao, H.; Huang, Z.; Ren, X.; Liu, S.; Zhang, Y.; Qi, X.; Zhang, H., Self-Powered Photodetectors Based on 2D Materials. *Advanced Optical Materials* **2020**, 8 (1), 1900765.
- [3] Lorenz, T.; Ghorbani-Asl, M.; Joswig, J. O.; Heine, T.; Seifert, G., Is MoSe₂ a robust material for 2D electronics? *Nanotechnology* **2014**, 25 (44), 445201.
- [4] Novoselov, K. S.; Mishchenko, A.; Carvalho, A.; Castro Neto, A. H., 2D materials and van der Waals heterostructures. *Science* **2016**, 353 (6298), aac9439.
- [5] Mondal, D.; Sharma, D.; R, K.; N, A. M.; Tiwary, C. S.; Bhat, N.; Kamble, V. B., Native Oxide MoO₂- MoSe₂ Heterostructure-Based Self-Powered Gas Sensor for Selective NO₂ and H₂ Detection. *Small* **2025**, 21 (33), 2503284.