Operando Investigation of WS_2 Gas Sensors: Simultaneous Ambient Pressure X-ray Photoelectron Spectroscopy and Electrical Characterization coupled to theoretical modelling[1]

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Novel two-dimensional (2D) materials beyond graphene, particularly transition metal dichalcogenides (TMDs) such as WS_2 and MoS_2, have gained significant attention due to their potential for developing highly sensitive, selective, and low-power gas sensors operating at room temperature. A deeper understanding of the adsorption properties of these layered 2D materials is essential for optimizing the design and fabrication of advanced sensing devices. In this context, accurately predicting and determining the adsorption process of semiconductor-based 2D sensors is a key step toward improving their technological performance and reliability. To address this challenge, we combine theoretical and experimental approaches. First-principles (DFT) calculations are employed alongside ambient-pressure X-ray photoelectron spectroscopy (AP-XPS) measurements to quantify the sensitivity of layered semiconducting TMDs (MX_2 systems) toward specific gas molecules such as NH_3 and NO_2. DFT computations are used to analyze the relative core-level shifts induced by changes in the chemical environment at the MX_2/gas interface (i.e., identifying gas analytes interacting with MX_2) as well as by structural modifications within MX_2 (i.e., the introduction of defects to enhance gas-sensing performance). Theoretical modeling using DFT enabled us to identify opposing behaviors in terms of detection mechanisms, particularly with regard to electrostatic effects (i.e., energy shift of the MX_2 work function), and also to explain why we observed greater charge transfer for one type of molecule than for another. All of this was initially carried out in the pristine case. We also studied the following cases: a material with a sulfur defect and one where we replaced the sulfur vacancy with an oxygen atom. This theoretical study ultimately enabled us to highlight a type of MX_2 system interacting with NO_2 and NH_3 and to correlate the theoretical study with the experimental study based on resistivity and XPS measurements.

References

[1] SCARDAMAGLIA, Mattia, CASANOVA-CHÁFER, Juan, TEMPERTON, Robert, *et al.* Operando Investigation of WS2 Gas Sensors: Simultaneous Ambient Pressure X-ray Photoelectron Spectroscopy and Electrical Characterization in Unveiling Sensing Mechanisms during Toxic Gas Exposure. *Acs Sensors*, 2024, vol. 9, no 8, p. 4079-4088.