Ab initio study of ultrasensitive H_2S gas sensors based on WS_2 hybrid materials

José J. Baldoví, Alejandro Pérez Paz, Lede Xian, Krisztian Kordas, Ángel Rubio
Max Planck Institute for the Structure and Dynamics of Matter,
Luruper Chaussee 149, Hamburg, Germany
jose.baldovi@mpsd.mpg.de

Gases with different properties, origins, and concentrations are pervasive in our environment. Some of these gases are highly toxic and hazardous, while others are essential for life or indicators of health status. Accordingly, sensors for gas detection and monitoring are needed in various sectors such as environmental protection, industrial process monitoring and safety, amenity, energy saving, health, and food industries. [1] Metal oxide semiconductors stand out as the most common active sensing materials used in practical devices. Among the new types of nanoscopic sensors being studied, layered transition metal dichalcogenide (MX2, M = Mo, W; X = S, Se) nanostructures have recently attracted significant interest. Often compared to graphene and other two-dimensional (2D) nanomaterials, their properties present distinct advantages for electronic, optical, and electrochemical sensors. [2]

In this contribution, we explore the gas sensing behavior of WS_2 nanowire-nanoflake hybrid materials that possess excellent sensitivity and high selectivity towards H_2S relative to CO, NH3, H2, and NO. Gas response measurements, complemented with the results of X-ray photoelectron spectroscopy analysis and *first principles* calculations based on density functional theory, suggest that the intrinsic electronic properties of pristine WS_2 alone are not sufficient to explain the observed high sensitivity towards H_2S. A major role in this behavior is also played by O doping in the S sites of the WS_2 lattice. The results of the present study open up new avenues for the use of transition metal disulphide nanomaterials as effective alternatives to metal oxides in future applications for industrial process control, security, and health and environmental safety. [3]

References

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[3] Asres, G. A.; **Baldoví, J. J.**; Dombovari, A.; Järvinen, T.; Lorite, G. S.; Mohl, M.; Shschukarev, A.; Pérez Paz, A.; Xian, L.; Mikkola, J.-P.; Spetz, A. L.; Jantunen, H.; Rubio, A.; Kordas, K, *Nano Research*, 11 (2018) 4215.

Figures

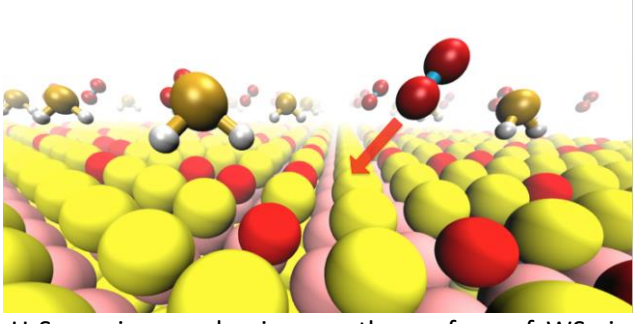

Figure 1: Art illustration of H_2S sensing mechanism on the surface of WS_2 in the presence of O_2. In the presence of air (O_2), the WS_2 lattice is doped with O, partially substituting S in the anionic sites.