Hydrogen Sensing Mechanism of WS_2 Gas Sensors Analyzed with NAP-XPS

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The successful deployment of green hydrogen technology is dependent on the use of affordable yet reliable hydrogen sensors throughout the entire process. From generation to transport/distribution, storage, and consumption, hydrogen sensors play a crucial role in ensuring the efficiency and safety of the hydrogen chain. For example, hydrogen sensors are needed at generation to help monitor and optimize the efficiency of the hydrogen evolution reaction (HER). They are also required to ensure the safe operation of the whole hydrogen chain. Indeed, H_2 is a small molecule that easily diffuses through materials and may leak from containers, especially when kept at high pressure (e.g., 900 bar). In addition, hydrogen is odorless and collects under roofs and overhangs, where it can generate explosion hazards.

Nanostructured tungsten disulfide (WS_2) is one of the most promising candidates for being used as an active nanomaterial in chemiresistive gas sensors, as it responds to hydrogen gas at room temperature. This study analyzes the hydrogen sensing mechanism of a nanostructured WS_2 layer using near-ambient-pressure X-ray photoelectron spectroscopy (NAP-XPS) and density functional theory (DFT). The W 4f and S 2p NAP-XPS spectra suggest that hydrogen makes physisorption on the WS_2 active surface at room temperature and chemisorption on tungsten atoms at temperatures above 150 °C. DFT calculations show that a hydrogen molecule physically adsorbs on the defect-free WS_2 monolayer while it splits and makes chemical bonds with the nearest tungsten atoms on the sulfur point defect. The hydrogen adsorption on the sulfur defect causes a large charge transfer from the WS_2 monolayer to the adsorbed hydrogen. In addition, it decreases the intensity of the in-gap state, which is generated by the sulfur point defect. Furthermore, the calculations explain the increase in the resistance of the gas sensor when hydrogen interacts with the WS_2 active layer.