

Engineering Selective Detection of Hazardous H₂ and NO₂ Using Pd Functionalized MXene/ WS₂ Gas Sensors

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Summary:

Reliable detection of hazardous gases such as hydrogen (H₂) and nitrogen dioxide (NO₂) is essential for industrial safety, environmental monitoring, and emerging hydrogen-based energy technologies. Two-dimensional transition metal dichalcogenides (TMDs), particularly WS₂, have recently garnered attention as promising materials for gas sensing applications, due to their high surface reactivity and tunable electronic properties. In this work, the sensing performance of WS₂ was engineered through hybridization with titanium carbide MXene (Ti₃C₂T_x) and palladium nanoparticles. This study presents a highly sensitive Pd functionalized MXene/WS₂ nanocomposite-based sensors operating at low temperature of 100 °C. The WS₂/MXene sensor exhibited a clear sensitivity toward NO₂, with a response of 75%. After Pd functionalization, the sensing behavior shifted from NO₂ toward H₂, giving a dominant H₂ response of approximately 66%, while the response toward NO₂ decreased to nearly half.

Keywords: Gas sensor, TMDs, MXene, nanomaterials, Palladium functionalization.

Background, Motivation and Objective

The development of highly sensitive and selective gas sensors is crucial for environmental monitoring and industrial safety. Nitrogen dioxide (NO₂) is a hazardous air pollutant linked to respiratory diseases, while hydrogen (H₂) is highly flammable and possesses significant explosion risks in hydrogen storage and fuel-cell systems. With the increasing adoption of hydrogen as a clean energy carrier, reliable detection of H₂ leaks has become particularly important for ensuring safe operation [1]. Two-dimensional (2D) materials have recently attracted considerable attention for gas sensing applications due to their high surface-to-volume ratio and tunable electronic properties. Among them, tungsten disulfide (WS₂), a transition metal dichalcogenide (TMD), has shown strong potential for gas detection owing to its edge-rich structure and high surface reactivity [2]. However, pristine WS₂ often exhibits limited selectivity. To address this limitation, hybrid material engineering strategies have been explored. MXenes such as Ti₃C₂T_x offer high electrical conductivity and abundant surface terminations, enabling the formation of conductive heterostructures with semiconducting sensing layers. Additionally, palladium (Pd) nanoparticles exhibit strong catalytic affinity toward

hydrogen through dissociation and spillover mechanisms, which can significantly enhance H₂ sensing performance [3]. In this work, two sensing platforms WS₂/MXene and WS₂/MXene/Pd were developed and compared to the pristine WS₂ to investigate how MXene integration and Pd decoration influence the sensing behavior and selectivity of WS₂-based gas sensors.

Materials and Methods

WS₂ was synthesized as reported in our previous study [2]. To fabricate the WS₂/MXene heterostructure sensor, 10 mg of previously synthesized WS₂ powder was dispersed together with 5 mg of Ti₃C₂T_x MXene in 10 mL of absolute ethanol. The mixture was ultrasonicated for 60 minutes to ensure homogeneous dispersion between the two materials. Subsequently, 3 mL of the obtained suspension was airbrushed onto an alumina substrate equipped with platinum interdigitated electrodes on the front side and a platinum resistive heater on the back side. For the preparation of the Pd-functionalized WS₂/MXene sensor (WS₂/MXene/Pd), the previously fabricated WS₂/MXene sensor was decorated with Pd nanoparticles using aerosol-assisted chemical vapor deposition (AACVD) as reported in our previous work [1].

Results

Fig. 1 (a, b) illustrates the FESEM images of the prepared WS₂/MXene and WS₂/MXene/Pd heterostructures respectively. The morphology analysis revealed that the WS₂/MXene heterostructure exhibits relatively smooth and flat flake-like domains, whereas the Pd-functionalized WS₂/MXene/Pd sample shows a noticeably rougher and more corrugated surface decorated with nanoscale protrusions. This morphological evolution is mainly attributed to the nucleation and growth of Pd nanoparticles during AACVD, which preferentially occurs at defects, edges, and active surface sites, thereby increasing the surface roughness and producing a less planar appearance. EDX mapping confirms the presence of MXene in both samples, indicated by the red color across the surface. In the Pd-modified sample, additional blue signals corresponding to Pd appear, confirming the successful decoration of the WS₂/MXene heterostructure with Pd nanoparticles as shown in Fig. 2 (a, b).

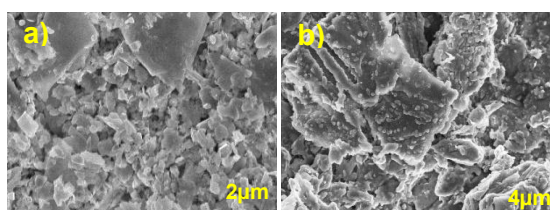


Fig. 1. FSEM images of (a) WS₂/MXene, (b) WS₂/MXene/Pd.

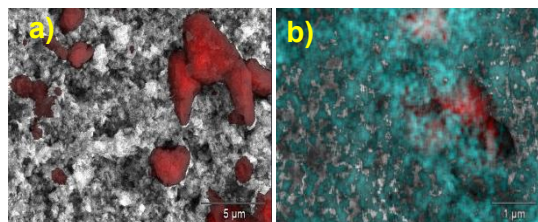


Fig. 2. (a) EDX mapping of WS₂/MXene, (b) EDX mapping of Pd decorated WS₂/MXene sensor.

The sensing performance of the fabricated sensors was compared with the pristine WS₂ sensor at different operating temperatures to identify the optimal working conditions. 100 °C provided the best discrimination between the target gases. Gas sensing measurements were therefore conducted toward 800 ppb NO₂ and 800 ppm H₂ at this temperature. Fig. 3(a, b) shows the dynamic resistance response of the sensors, while the corresponding response values are summarized in Fig. 4. The pristine WS₂ sensor exhibited responses of 48.69% toward NO₂ and 6.1% toward H₂. The WS₂/MXene heterostructure showed an enhanced response toward NO₂ (75.6%), indicating improved interaction due to MXene incorporation. In contrast, the WS₂/MXene/Pd sensor

displayed a significantly higher response toward H₂ (66.5%), while the response to NO₂ decreased to 36.8%. The detailed selectivity and humidity sensing responses will be presented at the conference.

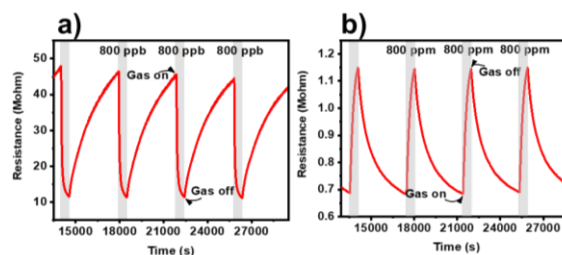


Fig. 3. Resistance dynamics of (a) WS₂/MXene towards 800 ppb NO₂, (b) WS₂/MXene/Pd toward 800 ppm H₂

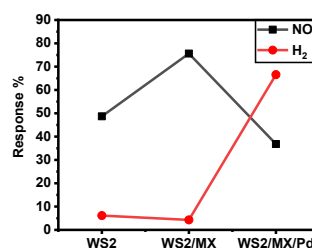


Fig. 4. (a) the sensors response towards NO₂ & H₂ at 100 °C.

Conclusions

This study demonstrates that MXene improves NO₂ sensing performance, whereas Pd functionalization shifts the selectivity toward H₂ gas.

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