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Light stimulation enhanced detection of NO at ppb-level at room temperature using $MoS_2/WSe_2/GaN$ heterostructure sensor

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Supporting Information:

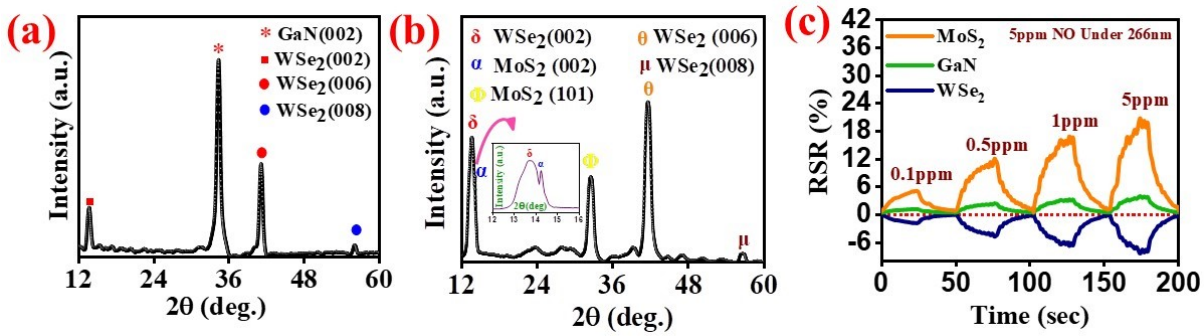

Fig S1. XRD Spectra of (a) WSe_2/GaN. (b) MoS_2/WSe_2 (c) Relative sensor response of bare MoS_2, WSe_2, and GaN for 5ppm NO under 266nm.

Characteristics peaks at 13.64°, 34.38°, 41.66°, and 56.68° appear in the pattern of XRD for WSe_2/GaN. The peaks at 13.64°, 41.66°, and 56.68° refer to the (002), (006), and (008) planes of WSe_2, respectively, corresponding to the formation of hexagonal WSe_2 according to JCPDS (38-1388). Besides, the peak at 34.46° confirms the GaN (002) plane. Additional diffraction peaks at 14.20° and 33.18° correspond to the (002) and (100) planes of MoS_2, while WSe_2 presents peaks at 13.48°, 41.65°, and 56.17° assigned to the (002), (006), and (008) planes of hexagonal WSe_2. From these results, both MoS_2 and WSe_2 were successfully grown in the heterostructure. Further, for the detection of 5 ppm NO under 266 nm illumination, the relative sensor response for pristine MoS_2, WSe_2, and GaN is much lower. In the case of pristine samples, there are limited active sites and weak adsorption/desorption kinetics that limit the gas-sensing performance. The pristine layers of MoS_2 and WSe_2 have a lesser number of active sites for adsorbing gases because they contain relatively inert basal planes; however, the layer of GaN, which contains strong ultraviolet absorption, is deficient in surface-interaction capabilities to detect NO appropriately.

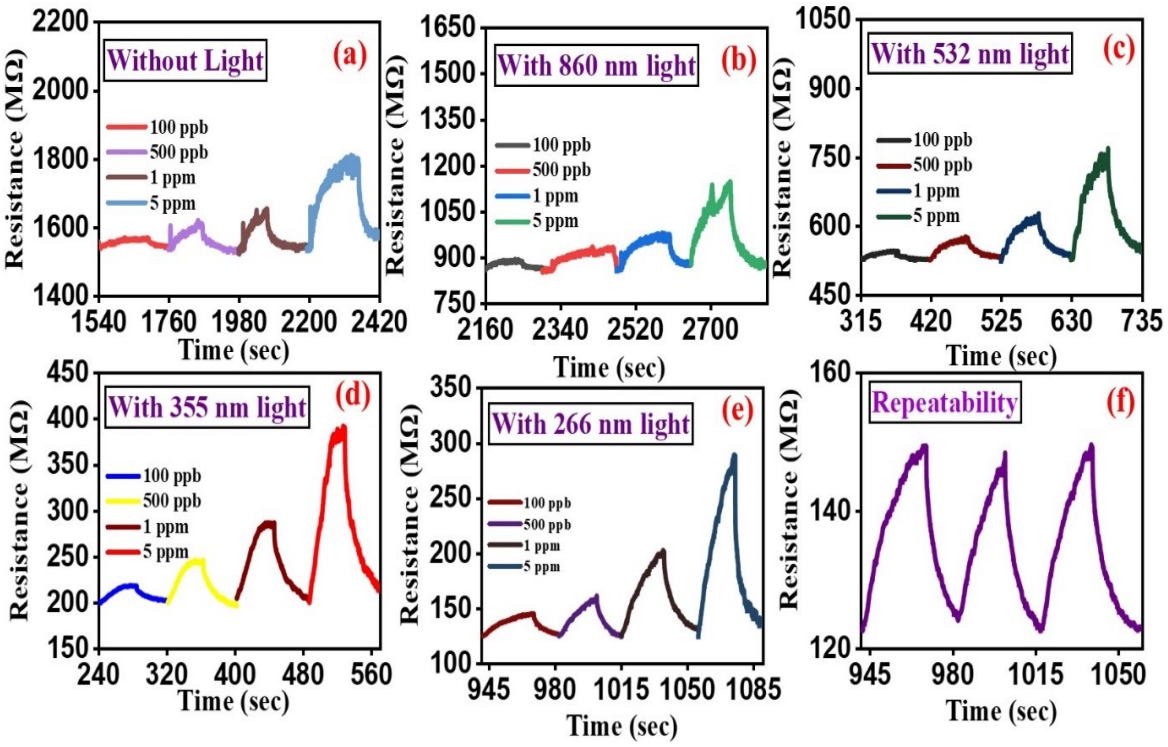

Fig S2. Dynamic resistance response of the prepared $MoS_2/WSe_2/GaN$ heterostructure sensor for NO gas sensing in different conditions: (a) dark, (b) 860 nm illumination, (c) 532 nm illumination, (d) 355 nm illumination, and (e) 266 nm illumination. The wavelength dependence of the sensor system's response is observed to be sensitive toward lower wavelengths. (f) The reproducibility curve for 100 ppb NO detection under 266 nm light illumination demonstrates the measurement's stability and repetition.

It has been seen that the dynamic resistance response of the $MoS_2/WSe_2/GaN$ heterostructure sensor to NO gas sensing under varying illumination is influenced by the interaction between light and the electronic structure of the material, and an increase in sensitivity with decreasing wavelength of illumination, peaking at 266 nm. The photoexcitation, band alignment, and kinetics of gas adsorption control such behavior. At shorter wavelengths, the sufficient energy of photons facilitates multiple electron-hole pair generation, which elevates the carrier density and photoconductive response. The band alignment enables the extension of charge separation into greater carrier lifetimes and the transfer of charges toward NO molecules upon illumination with UV. Higher carrier generation at 266 nm also enhances sensitivity by maximizing gas-surface interactions and accelerating the desorption of gases; the response and recovery times also rise. The sensor is highly responsive to NO gas due to this synergistic effect of photon energy and charge carrier dynamics under UV illumination.