Chemical Sensing by Band Modulation of a Black Phosphorus/Molybdenum Diselenide van der Waals Heterostructure

Zhihong Feng, Daihua Zhang

College of Precision Instrument and Opto-electronics Engineering, Tianjin University, Tianjin 300072, China <u>zhfeng@tju.edu.cn</u>

Abstract

Van der Waals heterostructures based on two-dimensional (2D) materials have attracted considerable research interest in the past few years. In contrast to conventional heterostructures formed by covalent bonds that are generally associated with atomic/ionic inter-diffusion, the van der Waals heterostructure has an abrupt transition between the two materials and a sharp gradient of carrier concentration across the interface¹. Their unique structural and physical properties have enabled new possibilities for a large array of novel devices and applications ranging from vertical tunneling transistors², barristors³ to optoelectronic applications⁴. However, few have investigated their interaction with gaseous molecules and application as chemical or biological sensors.

In this work, we demonstrate a van der Waals heterostructure chemical sensor based on few-layered black phosphorus (BP) and molybdenum diselenide (MoSe₂) flakes. Due to the atomically thin nature of 2D materials, surface adsorption of gas molecules can effectively modulate the band alignment at the BP/MoSe₂ interface and, correspondingly, the electron transport characteristics of the device, making it a highly sensitive detector for chemical and physical adsorptions. Compared with sensors made of homogeneous nanomaterials on the same substrate, our device demonstrates a marked enhancement in detection limit and sensitivity by orders of magnitude for NO₂ detection. Kelvin probe force microscopy (KPFM) analysis confirms that the total built-in potential at the hetero-interface dramatically increases after exposure of NO₂ and provides direct evidence of the changes in band alignment due to NO₂ adsorption. Finite element model based on the quantitative KPFM results reveals that the modulation of barrier height in MoSe₂, which is induced by the modulation of both the total built-in potential and the ratio between majority carrier concentrations of both materials, is responsible for the enhanced sensitivity. Our work demonstrates the potential of van der Waals heterostructure as a fundamentally new platform for sensing applications and also provides insights into the interactions between gaseous molecules and 2D heterostructures.

References

[1] Fang, H. et al. Proc. Natl. Acad. Sci. U. S. A. 111(2014), 6198–202.

- [2] Britnell, L. et al. Science 335(2012), 947–950.
- [3] Yang, H. et al. Science 336(2012), 1140-1143.
- [4] Xia, F. et al. Nat. Photonics 8(2014), 899–907.

Figures



(a) Optical image of the fabricated device. The green flake is multi-layered BP, while the dark blue flakes are few-layered $MoSe_2$. Scale bar, 15 μ m. (b) Gate tunable I-V characteristics of the BP/MoSe₂ hetero-junction. Inset: I-V characteristics under semilog scale. (c) Response of all three sensors as a function of gas concentration under logarithm scale. The intersection between each fitting line and the horizontal 3% SNR threshold (blue dashed line) corresponds to the detection limit of each sensor.