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## Preparation and mechanism of molybdenum diselenide nanosheets for ethanol detection

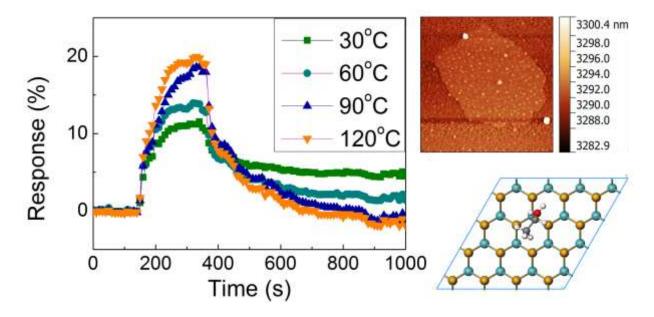
Two-dimensional (2D) transition metal dichalcogenides (TMDCs) as alternative sensor materials of conventional metal oxides have attracted much attention recently [1,2]. These materials present enormous surface/volume ratio and unusual electronic, optical, and magnetic properties in the form of single- or few-layer, and have accelerated the development of a diverse range of applications including gas sensor [3]. Among TMDCs, molybdenum diselenide (MoSe<sub>2</sub>), as an emerging semiconducting material has rarely been investigated for sensor application. Late et al. firstly investigated the mechanically exfoliated single-layer MoSe<sub>2</sub> and demonstrated its high sensing performance to ppm-level NH<sub>3</sub> gas [4]. Very recently Baek et al. also developed a MoSe<sub>2</sub> multilayer based field-effect transistor (FET) for detecting NO<sub>2</sub> gas [5]. However, the sensing mechanism of ultrathin MoSe<sub>2</sub> is still ambiguous to date.

In this study, MoSe<sub>2</sub> nanosheets thin film gas sensor was firstly fabricated and its sensing potential to ppm-level ethanol vapor at low operating temperature was investigated. Ultrathin MoSe<sub>2</sub> nanosheets were prepared in large scale through a facile liquid-phase exfoliation method using low boiling temperature solvent. The exfoliated MoSe<sub>2</sub> nanosheets exhibited high purity and crystallinity with few atomic layer thickness. Systematical gas sensing tests demonstrated that MoSe<sub>2</sub> nanosheets based thin film could be utilized as ethanol gas sensor with linear response, quick recovery, and good repeatability at 90°C, as shown in Figure 1. The sensing mechanism of MoSe<sub>2</sub> toward ethanol was investigated based on first principle calculation. The adsorption behavior of ethanol molecule on MoSe<sub>2</sub> surface was revealed in light of adsorption orientation, adsorption energy, charge transfer, projected electronic density of state, and molecular orbital. The calculation well matched with experimental results. It is found the quick and complete recovery of MoSe<sub>2</sub> nanosheets sensor were benefited by the appropriate physical interaction between ethanol and MoSe<sub>2</sub> surface. This finding offers a competitive option instead of conventional graphene sensor for ethanol gas detection at low temperature.

## References

- [1] B. L. Li, J. P. Wang, H. L. Zou, S. Garaj, C. T. Lim, J. P. Xie, N. B. Li, and D. T. Leong, Adv. Funct. Mater., 26 (2016) 7034.
- [2] J. H. Cha, S. J. Choi, S. Yu, and I. D. Kim, J. Mater. Chem. A, 5 (2017) 8725.
- [3] W. Choi, N. Choudhary, G. H. Han, J. Park, D. Akinwande, and Y. H. Lee, Mater. Today, 20 (2017) 116.
- [4] D. J. Late, T. Doneux, and M. Bougouma, Appl. Phys. Lett., 105 (2014) 233103.
- [5] J. Baek, D. Yin, N. Liu, I. Omkaram, C. Jung, H. Im, S. Hong, S. M. Kim, Y. K. Hong, J. Hur, Y. Yoon, and S. Kim, Nano Res., 10 (2017) 1861.

## Figures



**Figure 1:** Typical sensing response curves of MoSe<sub>2</sub> nanosheets sensor toward 20 ppm ethanol with different operating temperatures (left). AFM image of as-prepared MoSe<sub>2</sub> nanosheet (upper right). Adsorption model of ethanol molecule on MoSe<sub>2</sub> surface (lower right).