



High-Concentration Niobium-Substituted WS₂ Basal Domains with Reconfigured Electronics Band Structure for Hydrogen Evolution Reaction

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Abstract:

Transition metal dichalcogenides (TMDCs) monolayers have attracted intense interests owing to their unique layer-dependent electrical and optical properties, electrocatalytic active properties, and crystal structure tunability, which show great potential for electronics, optoelectronics, valleytronics, spintronics and catalysis applications.¹⁻⁵ However, the field effect transistors based on layered TMDCs is often plagued by issues such as low field effect mobility and low on/off current ratio due to the high contact resistance at the 2D-semiconductor/bulk-metal interface.^{4,5} Recent efforts based on phase transition surface molecular doping, and in-situ atomistic substitutional doping in 2D semiconductors have been shown to allow enhanced control of the types of majority charge carriers and also to achieve modulation of their band structure, which are the key steps towards high-performance 2D-semiconductor-based electronics, optoelectronics and electrocatalysis devices.⁶⁻⁹ However, an in-situ transition metal doping strategy for uniform and large-area chemical vapor deposited 2D semiconductors remains a formidable challenge. Here we synthesize highly uniform niobium substituted tungsten disulfides (Nb-WS₂) monolayer, with a doping concentration of nearly 7 % and sizes reaching 100 μm, through a metal dopant precursor route, using salt-catalyzed chemical vapor deposition (CVD). Our results reveal unusual effects in the structural, optical, electronic and electrocatalysis characteristics of Nb-WS₂ monolayer. The Nb dopants readily induce a band restructuring effect, providing the most active site with a hydrogen adsorption energy of 0.175 eV. The combined advantages of the unusual physics and chemistry by in-situ CVD doping technique open the possibility in designing 2D-material-based electronics and catalysts of novel functionalities.

Biography:

Pam Mei Er received her bachelor's degree from the University of Malaya, Malaysia in 2016. She is currently a Ph. D candidate under supervision of Assistance Professor Yang Hui Ying in the Engineering Product Development Pillars at the Singapore University of Technology and Design, Singapore. Her current research mainly focuses on the chemical vapor deposition synthesis of atomically thin layer transition metal dichalcogenides



based materials and the investigation of their potential electrochemical applications.

Publication of speakers:

- Miyauchi, Y.; Konabe, S.; Wang, F.; Zhang, W.; Hwang, A.; Hasegawa, Y.; Zhou, L.; Mouri, S.; Toh, M.; Eda, G.; Matsuda, K. 2018, Evidence for Line Width and Carrier Screening Effects on Excitonic Valley Relaxation in 2D Semiconductors. *Nat. Commun.* 9; 2598.
- Tian, H.; Chin, M. L.; Najmaei, S.; Guo, Q.; Xia, F.; Wang, H.; Dubey, M. 2016, Optoelectronic Devices based on Two-dimensional Transition Metal Dichalcogenides. *Nano Res.* 9; 1543-1560.
- Jaramillo, T. F.; Jørgensen, K. P.; Bonde, J.; Nielsen, J. H.; Horch, S.; Chorkendorff, I. 2007, Identification of Active Edge Sites for Electrochemical H₂ Evolution from MoS₂ Nanocatalysts. *Science* 317; 100-102.
- Voiry, D.; Yang, J.; Chhowalla, M. 2016, Recent Strategies for Improving the Catalytic Activity of 2D TMD Nanosheets toward the Hydrogen Evolution Reaction. *Adv. Mater.* 28; 6197-6206.
- Cui, C.; Xue, F.; Hu, W.-J.; Li, L.-J. 2018. Two-dimensional Materials with Piezoelectric and Ferroelectric Functionalities. *npj 2D Mater. Appl.* 2; 18.
- Zhu, J.; Wang, Z.; Yu, H.; Li, N.; Zhang, J.; Meng, J.; Liao, M.; Zhao, J.; Lu, X.; Du, L.; Yang, R.; Shi, D.;

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