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Layered solids: from lubricants to 2D electronic materials*

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Abstract

Transition metal dichalcogenides (TMDs) with the chemical composition MX_2 (M=Mo,Ti and X=S,Se) are layered solids known for their excellent behavior as dry lubricants. Interestingly, TMDs have also caught strong interest from the post-graphene 2D electronics community, since they can be mechanically exfoliated down to monolayer thickness, becoming direct-gap semiconductors. Initial quantum trasport measurements have suffered from limitations imposed by conventional contact materials such as Au [1]. In retrospect, this makes sense, since 'nothing should stick to a lubricant'. Only after a long search, optimum strategies have been devised to make low-resistance, ohmic contacts to TMDs [2] using similar, epitaxial TMDs. A second problem in optoelectronic applications of TMDs arises from using CVD as a scalable growth process, which produces highly defective material. Defects such as chalcogen vacancies scatter charge carriers and quench photoluminescence. Recent experimental and theoretical [3] studies suggest that exposure of defective MoS_2 to sulfur-containing compounds may effectively heal such defects. Predictive *ab initio* calculations provide useful guidance to experimental studies in this case.

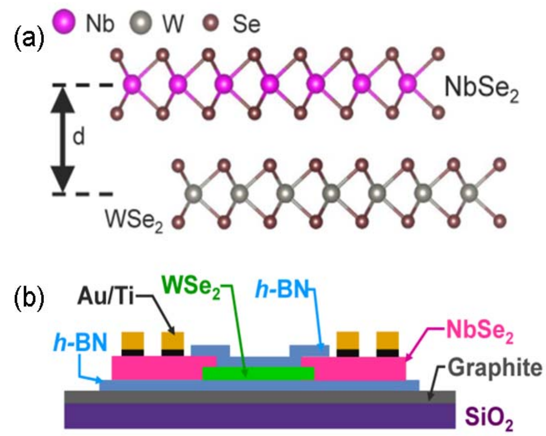

FIG.1. WSe_2 field-effect transistor with conducting $NbSe_2$ leads in side view. Atomic-model representation of the $NbSe_2/WSe_2$ interface (top) and schematic structure of the device (bottom). (From Ref. [2]).

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References:

[1] Igor Popov, Gotthard Seifert, and David Tománek, Phys. Rev. Lett. **108**, 156802 (2012).
[2] Jie Guan, Hsun-Jen Chuang, Zhixian Zhou, and David Tománek, ACS Nano **11,** 3904 (2017).
[3] Anja Förster, Sibylle Gemming, Gotthard Seifert, and David Tománek, ACS Nano **11** (2017).