Improving the Functionality of Atomically Thin Layered Materials

Achievement: Large-area “in situ” transition-metal substitutional doping via thermal chemical-vapor deposition of semiconducting transition-metal-dichalcogenide monolayers deposited on dielectric substrates.

Significance and Impact: This work enables stable transition-metal substitution that preserves the monolayer’s semiconducting nature, along with other characteristics, including direct bandgap photoluminescence. Such tuning of functionality achieves one major prerequisite for integration into modern solid-state electronic and optoelectronic technology.

Research Details:
- Aberration-corrected scanning transmission electron microscopy (STEM) to analyze the crystal structure and doping
- First principles calculations based on density functional theory to understand the effect of substitutional doping
- A scalable one-pot thermal CVD synthesis approach

Sponsor/Facility: N.K. acknowledges funding support from the USA National Science Foundation (Award Numbers: 1435783, 1510828 and 1608171), New York State under NYSTAR program C080117, and from the John A. Clark and Edward T. Crossan Endowed Chair Professorship at the Rensselaer Polytechnic Institute (RPI). The theoretical work was also supported in part by the Office of Naval Research. The computations were performed using the resources of the Center for Computational Innovation at RPI. L.L. was supported as a Eugene P. Wigner Fellow at Oak Ridge National Laboratory. J.H. and Y.D.K. acknowledge support from the NSF MRSEC program through Columbia in the Center for Precision Assembly of Superstratic and Superatomic Solids (DMR-1420634). Microscopy research was conducted as part of a user proposal through ORNL’s Center for Nanophase Materials Sciences, which is a U.S. Department of Energy, Office of Science User Facility (J.C.I.).

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Publication: “Transition-Metal Substitutional Doping in Synthetic Atomically Thin Semiconductors” Jian Gao, 1 Young Duck Kim, 2 Liangbo Liang, 3,4 Juan Carlos Idrobo, 4 Phil Chow, 1 Jiawei Tan, 1 Baichang Li, 1 Lu Li, 5 Bobby G. Sumpter, 4 Toh-Ming Lu, 3 Vincent Meunier, 3 James Hone, 2 Nikhil Koratkar 1 Adv. Mater. (2016) DOI: 10.1002/adma.201601104

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Overview:
As device length scales progressively shrink, they push the limits of silicon technology, and new challenges emerge that must be addressed to meet this requirement. The family of layered semiconductors, known as the transition metal dichalcogenides (TMDCs), represents one such alternative that has met a surge of recent interest for optoelectronics applications due to attractive physical scaling properties and exotic behavior in the atomically thin regime. However appropriate doping and control has been largely lacking. In this work, we successfully demonstrate large-area “in situ” transition-metal doping for synthetic TMDC monolayers achieved by doped atomically thin WS$_2$ and MoS$_2$ monolayers with niobium (Nb) and rhenium (Re) impurities during the CVD-growth process. This method is based on a thermal chemical vapor deposition (CVD) approach that entails a scalable one-pot synthesis procedure. Detailed characterization and theoretical modeling show that the situ doping of transition-metal atoms during the growth of chemical vapor deposited monolayer MoS$_2$ and WS$_2$, leave the direct-gap semiconductor behavior of the atomically thin materials intact. Thus our results showcase a powerful doping strategy for altering the electronic behavior of atomically thin, chemical vapor deposited TMDCs by substitutional doping of the transition-metal atoms with impurity transition metals.