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Composition-Gradient-Mediated Semiconductor–Metal Transition in Ternary Transition-Metal-Dichalcogenide Bilayers

The semiconductor–metal transition (SMT) enables multiple applications of one single material, especially in modern devices. How to control it remains one of the most intriguing questions in material physics/chemistry, especially in two-dimensional layered materials. In this work, we report realization of SMT in MoS2–xOx bilayers, driven by the concentration gradient of the chalcogen atom across the van der Waals (vdW) gap of the disordered bilayers. Using the cluster expansion method, we determined that either semiconducting (stable) or metallic states (metastable) can be realized in MoS2–xOx bilayers with the same composition. Machine learning analysis revealed that the concentration gradient of the chalcogen atom across the vdW gap is the leading fingerprint of SMT, with structural distortion induced by atom mixing being a significant secondary factor. The electronic origin of the SMT is the broadening of the Mo dz2 and O pz bands, accompanied by the redistribution of the d electrons. This in-vdW-gap composition-gradient-driven SMT phenomenon also applies to MoSe2–xOx and MoTe2–xOx bilayers. The present work provides an alternative mechanism of SMT and demonstrates that the composition gradient across the vdW gap in the bilayer materials can be another degree of freedom to tune the band gaps without introducing extrinsic elements. Our findings will benefit the material design for small-scale and energy-efficient electronic devices.

Primary author: Mr CHEN, Qifan (Institute of Physics of the Czech Academy of Sciences)

Co-authors: Mr CHEN, Mingwei (Beihang University); Prof. ZHU, Linggang (Beihang University); Prof. MIAO, Naihua (Beihang University); Prof. ZHOU, Jian (Beihang University); Prof. ACKLAND, Graeme.J (University of Edinburgh); Prof. SUN, Zhimei (Beihang University)

Presenter: Mr CHEN, Qifan (Institute of Physics of the Czech Academy of Sciences)

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