Electronic structures of 2D transition metal dichalcogenides studied by angle-resolved photoemission

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Distinct properties of two-dimensional (2D) materials under quantum confinement are often governed by the changes in the electronic band structure and the lattice symmetry, and most pronounced in their single layer limit. Angle-resolved photoemission spectroscopy (ARPES) is a direct tool to investigate the underlying changes of band structure to provide essential information for understanding and controlling such properties.

Using the molecular beam epitaxy (MBE), we have been successfully growing 2D atomic layers of transition metal dichalcogenides (TMDs) with layer-by-layer thickness control. In situ synchrotron ARPES measurements reveal the details of the electronic structure evolution in these films. We have directly visualized the indirect-direct band gap transition in 2H-$MoSe_2$ and WSe_2, with significant spin splitting in the valence bands [1]. The charge density wave (CDW) orders in 2H-$NbSe_2$ and $TaSe_2$ are found to be persistent [2]. While they retain 3 x 3 ordering vector, the CDW transition temperatures stay virtually the same. We have also identified signatures of quantum spin Hall insulator, or 2D topological insulator, in the electronic structure of monolayer 1T'-WTe_2 [3].

References

[1] Y. Zhang *et al.*, Nature Nanotechnology **9** (2014) 111; Nano Letters **16** (2016) 2485.

[2] M. M. Ugeda *et al.*, Nature Physics **12** (2016) 92; H. Ryu *et al.*, Nano Letters (2018).

[3] S. J. Tang *et al.*, Nature Physics **13** (2017) 683; S. J. Tang *et al.*, APL Materials **6** (2018) 026601.

Figures

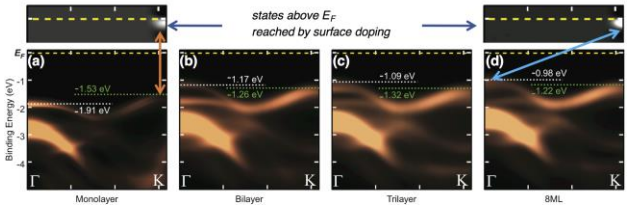

Figure 1: ARPES spectra of MBE grown 2H-$MoSe_2$ with (a) monolayer, (b) bilayer, (c) trilayer, and (d) 8-layer thicknesses.

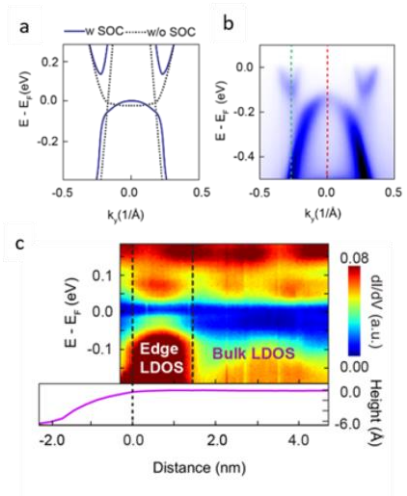

Figure 2: (a) Calculation and (b) ARPES spectra show the bulk gap opening due to a strong spin-orbit coupling in monolayer 1T'-WTe_2. (c) Spatial STS mapping across the edge of a 1T'-WTe_2 domain observes the edge state inside the bulk gap.