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Unravelling Electronic Band Structures of Transition Metal Dichalcogenides CHENDONG ZHANG, YUXUAN CHEN, AMBER JOHNSON, Univ of Texas, Austin, MING-YANG LI, JING-KAI HUANG, IAMS, Academia Sinica, LAIN-JONG LI, IAMS, Academia Sinica ; KAUST, CHIH-KANG SHIH, Univ of Texas, Austin — Accurate knowledge of the electronic structures of materials is the key enabler for the advancement of science and technology based on such materials. Recent emergence of transition metal dichalcogenides (TMDs) as potentially transformative 2D electronic and photonic materials has triggered intensive research activities to investigate their electronic structures. Compared with the previous experimental efforts such as optical spectroscopies and angle resolved photoemission, the scanning tunneling spectroscopy (STS) has the unique advantages in probing the quasiparticle band structures of the TMD samples with a limited lateral size. However, the STS investigations thus far have not yield consistent results even for the measurement of the quasiparticle band gap. Here we present a new comprehensive methodology of scanning tunneling spectroscopy, which contains the ability not only to probe electronic structures, but also to extract the information on their origins in the Brillouin zone. Thus, we map out, for first time, the critical point energy locations in both the valence and conduction bands of TMD compounds. This capability also allows us to unravel the systematic trend in the critical point energy locations as a function of the cation-anion orbital coupling, the spin-orbital coupling, as well as the interlayer coupling. Such knowledge is critical for the flourishing field of TMDs as emerging atomically thin 2D electronic and photonic materials.

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