Unlocking Mott correlations in 1*T*-TaS_2 with uniaxial strain

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Uniaxial strain offers a powerful route to study the interplay between the lattice and electronic correlations, revealing new insights into long-standing problems. One such enduring challenge is the controversial Mott phase in 1*T*-TaS_2, which has been debated for almost 50 years and has again recently been under intense scrutiny [1-4]. The phase diagram of this layered material is particularly rich, including charge density wave (CDW) phases, superconductivity under pressure, and a metastable phase following pulsed excitation. The existence of Mott behavior and the role of correlations was challenged when it was shown that interlayer hybridization could open a bonding-antibonding gap between bilayers of TaS_2 [1], leaving correlations ineffective. However, scanning tunneling microscopy (STM) data revealed that bilayers split by surface termination also display a gapped spectra [2,4], which implies the importance of correlations in the absence of the strong hybridization. Strain provides a route to modify the interlayer hybridization in order to test this hypothesis.

We used angle-resolved photoemission spectroscopy (ARPES) to probe the electronic structure in uniaxially-strained 1*T*-TaS_2 [5]. Following the application of strain, we observe a bandwidth-driven insulator-metal transition with reducing temperature. The presence of an emergent quasi-particle peak at the Fermi level indicates that the system hosts Mott correlations, which is further confirmed by our advanced electronic structure calculations (*GW*+EDMFT) performed for a split-bilayer terminated surface [6]. Our calculations further reveal that the correlated metal phase appears under strain due to a modification of interlayer coupling, realized by a change in the bulk stacking arrangement in the strained crystal. The observation of a strain-induced transition in 1*T*-TaS_2 may provide a route to understanding and controlling superconductivity and the pulse induced metastability that occur in this material.

References

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