Highlights

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Layer-dependent quantum cooperation of electron and hole states in the anomalous semimetal WTe_2

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Boosted by the anomalous bulk properties of semimetallic WTe2, here we report angle- and spin-resolved photoemission spectroscopy of WTe2 single crystals, through which we disentangle the role of W and Te atoms in the formation of the band structure and identify the interplay of charge, spin and orbital degrees of freedom. Supported by first-principles calculations and high-resolution surface topography, we reveal the existence of a layer-dependent behaviour. The balance of electron and hole states is found only when considering at least three Te–W–Te layers, showing that the behaviour of WTe2 is not strictly two dimensional.

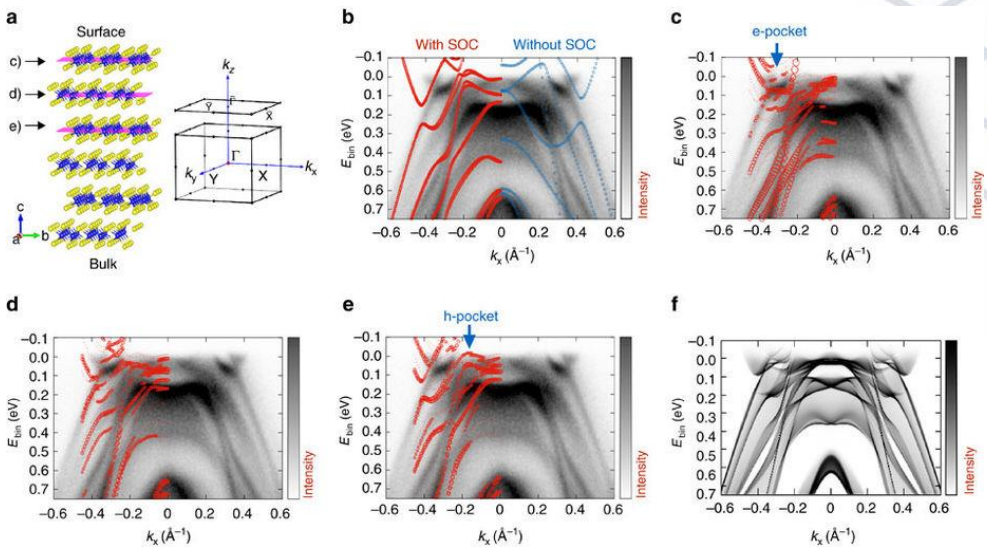

Figure 1. Evolution of band structure with number of layers. (a) Crystal structure of WTe2 with the bulk and surface Brillouin zones on the right. (b–e) ARPES measurements (hv.68 eV, T.77 K) of the electronic structure along the GX high symmetry direction (along the W-chains); (b) bulk electronic structures as calculated with spin-orbit coupling (SOC) (red bands at negative momenta) and without SOC (blue bands at positive momenta); theoretical bands projected (c) on the topmost WTe2 planes and (d,e) on second and third plane, respectively. In c,e, blue arrows mark the positions of the theoretical electron and hole pockets, respectively. In b,e, the size of the circles is proportional to the weight of the layer-resolved orbital character. (f) Theoretical surface spectral function A(k,E).