Emergent quantum size effects at topological insulator surfaces

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Bismuth-chalcogenides are model examples of three-dimensional topological insulators. Their ideal bulk-truncated surface hosts a single spin-helical surface state, which is the simplest possible surface electronic structure allowed by their non-trivial $Z_2$ topology. However, real surfaces of such compounds, even if kept in ultra-high vacuum, rapidly develop a much more complex electronic structure\(^1\) whose origin and properties have proved controversial. Here we demonstrate that a conceptually simple model, implementing a semiconductor-like band bending in a parameter-free tight-binding supercell calculation, can quantitatively explain the entire measured hierarchy of electronic states.\(^2\) In combination with circular dichroism in angle-resolved photoemission experiments, we further uncover a rich three-dimensional spin texture of this surface electronic system, resulting from the non-trivial topology of the bulk band structure. Moreover, our study sheds new light on the surface-bulk connectivity in topological insulators, and reveals how this is modified by quantum confinement.

\(^2\)M.S. Bahramy, P.D.C. King et al., Nature Commun. 3 (2012) 1159