New data suggests Si(111) 7x7 surface is not metallic

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Video Abstract

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Abstract

It took scientists more than 25 years to work out the structure of silicon's 7x7 surface reconstruction. Since reaching that milestone, experimental and theoretical studies have supported that this reconstruction produces a conductive, metallic surface. But new data gathered by an international team of researchers from Spain, the Philippines, France, and the United Kingdom say otherwise—a contradiction that could have technological implications for the integration of 2D silicon into electronic devices. The most widely accepted picture of silicon 111 's 7x7 surface reconstruction is the so-called dimer-adatom-stacking fault model. Here, dangling bonds produced by cleaving the bulk crystal occur on silicon adatoms, which are bonded to underlying bulk-silicon atoms, and on rest atoms in the lower layer. The rearrangement of charge associated with this structure produces an odd number of electrons, which implies that the surface should be metallic. Band structure measurements lead to a similar conclusion. They suggest the emergence of two itinerant surface states, S1 and S2, in the bulk band gap—with S1 believed to straddle the Fermi level closely enough to produce metallic behavior. But does it really? If the S1 state **_does_** cross the Fermi level of the 7x7 surface, the international team reported, then mapping the momentum of emitted photoelectrons as a function of the initial-state momentum would produce a map of the 2D Fermi surface itself. And mapping at different photon energies would essentially produce the same picture. But that's not what they observed. Using angle-resolved photoelectron spectroscopy, or ARPES, they found that this mapping produced three different angular patterns at three different photon energies. The upshot is that S1 and S2 are not itinerant band states but are actually localized to the adatoms and the rest atoms of the 7x7 surface. They do not cross the material's Fermi level, lying well below, indicating that the surface is not metallic. The findings suggest that interference effects caused by photoelectron diffraction might be more important than previously thought. Integrating these findings with other emerging data could provide a more complete picture of the electronic properties of 2D silicon and possibly other quantum materials.