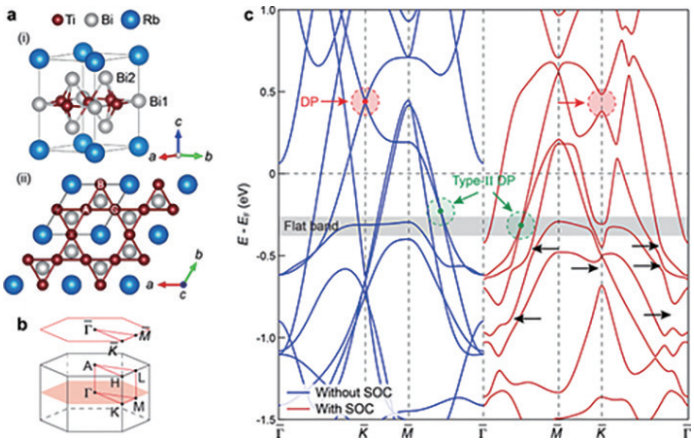
Basic Research

Scientists Reveal the Band Topology and Orbital-selective Nematicity in a New Ti-based Kagome Superconductor

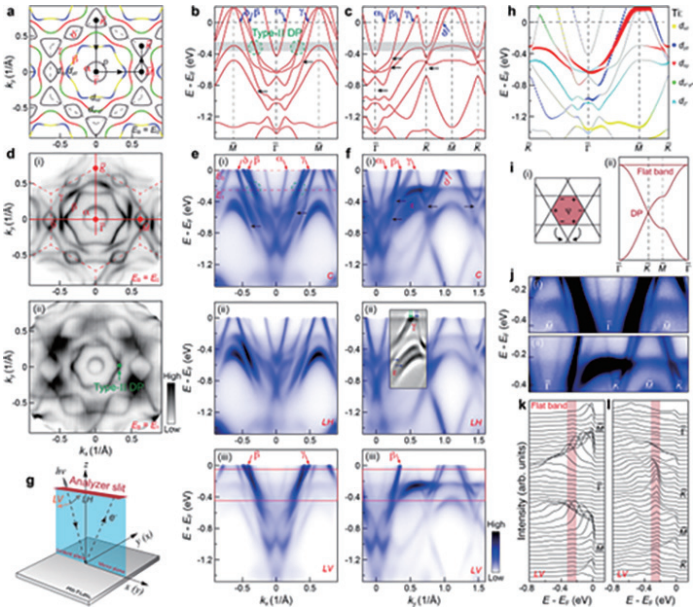
The kagome superconductor with a two-dimensional corner-sharing triangular lattice has attracted tremendous attention due to the interplay between nontrivial band topology, anomalous Hall effect (AHE), charge density waves (CDW), pair density wave (PDW), electronic nematicity and unconventional superconductivity. All these exotic quantum phenomena are thought to originate from the unique electronic structure of the kagome lattice including flat bands, Dirac cones and van Hove singularities. The flat band together with the van Hove singularities allows the system to remain in the strongly interacting regime. While, the Dirac cones promote non-trivial topology.

The kagome superconductor thus provides an excellent opportunity to study correlation-driven electronic states. Among them, electronic nematicity, commonly observed in juxtaposition with unconventional superconductivity, generates complicated superconducting pairing and intertwined electronic orders. Understanding the nature of the nematic state and its consequences for the electronic band structure and superconductivity has therefore become a key issue in kagome superconductors as well as high-temperature superconductors.

Nevertheless, in the present studies on kagome superconductor, the definitive identification of unique electronic structures is still scarce and the underlying mechanism to induce those exotic quantum phenomena from such electronic structures remains elusive. Meanwhile, identifying the driving force of electronic nematicity has been a central challenge for understanding nematicity. In iron-based superconductors, the problem is complicated because the spin, orbital and lattice degrees of freedom are intimately coupled. In AV_3Sb_5 kagome superconductors, the electronic nematicity



Crystal structure and calculated band structure of $RbTi_3Bi_5$. (Image by IOP)



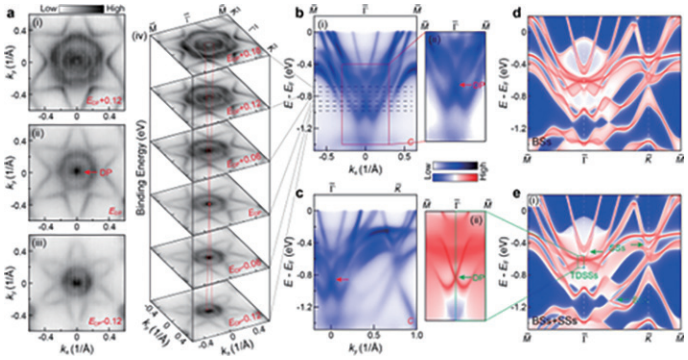
Polarization-dependent ARPES measurements of the kagome bands. (Image by IOP)

exhibits an intriguing entanglement with CDW, making understanding its origin difficult. Thus, to discover new kagome superconductors and explore the origins of CDW, PDW, electronic nematicity, and their correlation with unconventional superconductivity in this kagome system are of great significance.

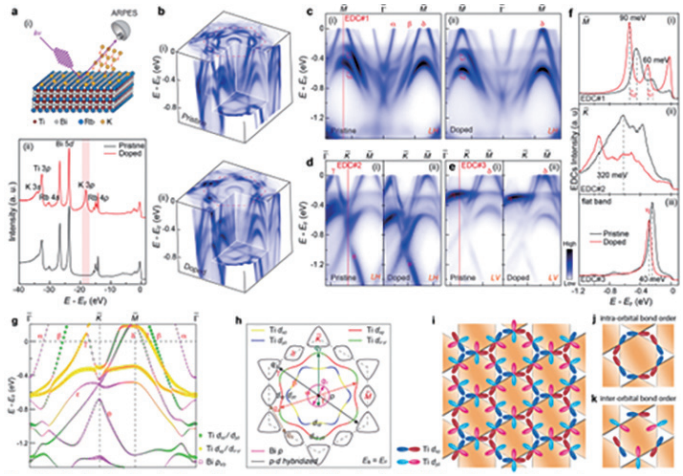
Recently, a team led by Prof. GAO Hongjun and Prof. YANG Haitao from the Institute of Physics (IOP), Chinese Academy of Sciences (CAS), in collaboration with SHI Ming's team from the Paul Scherrer Institute, Switzerland, and Prof. WU Xianxin from the Institute of Theoretical Physics, CAS, Prof. HU Jiangping and Prof. DONG Xiaoli from IOP, CAS, synthesized a new Titanium-based kagome superconductor, ATi_3Bi_5(A: Rb, Cs), and investigated the non-trivial band topology and orbital-selective electronic nematicity. The work entitled "Non-trivial band topology and orbital-selective electronic nematicity in a titanium-based kagome superconductor" was published in *Nature Physics*.

The Titanium-based kagome superconductor, ATi_3Bi_5(A: Rb, Cs), is a kagome superconductor prepared by Prof. GAO's team for the first time, and is isostructural to the AV_3Sb_5 superconductors (arXiv:2211.12264). Its crystal structure is formed by a succession of alternative stacking of the intercalated alkali-metal layer and the Ti_3Bi_5 layer that contains an ideal two-dimensional kagome lattice of Ti atoms coordinated by Bi atoms. In stark contrast to AV_3Sb_5, transport measurements on ATi_3Bi_5 show no evidence of a CDW state. Interestingly, an electronic nematicity with the rotational symmetry breaking is discovered in the absence of the concomitant translation symmetry breaking, similar to iron-based high-temperature superconductors. Therefore, ATi_3Bi_5 is a tantalizing system for understanding the mechanism behind electronic nematicity and its interplay with intertwined correlated quantum phenomena such as superconductivity.

The team firstly used the polarization-dependent angle-resolved photoemission spectroscopy to investigate the electronic structures of ATi_3Bi_5 single crystals. The strong spin-orbit coupling (SOC) from Bi atoms can generate intriguing nontrivial topological phenomena. The promising coexistence of flat bands, type-II Dirac nodal line and nontrivial Z_2 topological states is identified in $RbTi_3Bi_5$. Meanwhile, the team led by Prof. GAO, in collaboration with Prof. ZHOU Xingjiang's team at IOP, also directly identified the coexistence of



Z_2 topological surface states in $RbTi_3Bi_5$. (Image by IOP)



Orbital-selective doping effect and *d-p* hybridization in $RbTi_3Bi_5$. (Image by IOP)

a strikingly flat band, the type-II Dirac nodal loops, the type-III Dirac nodal loops and type-III Dirac nodal lines, and Z_2 nontrivial topological surface states formed from the band inversion due to strong SOC in $CsTi_3Bi_5$. This work entitled "Observation of flat band, Dirac nodal lines and topological surface states in Kagome superconductor $CsTi_3Bi_5$" was published in *Nature Communications*. The simultaneous existence of such multi-sets of nontrivial band structures in one kagome superconductor not only provides good opportunities to study related physics in the kagome lattice, but also makes ATi_3Bi_5 an ideal system to realize novel quantum phenomena by manipulating its chemical potential with chemical doping or pressure.

Remarkably, by working with doping-dependent ARPES via *in situ* surface potassium deposition, the team reveals the intricate orbital character change in $RbTi_3Bi_5$. Upon surface deposition, the electron doping in the kagome layers is mediated by the coupling between

Bi-*p* and Ti-*d* orbitals. This is the strongest *d*-*p* coupling, implying a strong inter-orbital coupling in the Ti-based kagome lattice in contrast to AV_3Sb_5. Meanwhile, the site symmetry is D_2h and thus all five orbitals on each site are non-degenerate, making the Ti-based kagome superconductor unique and distinct from iron-based superconductors. The revealed *d*-*p* hybridization, in conjunction with the inter-orbital coupling, breaks the six-fold rotational symmetry but preserves the two-fold rotational symmetry. It is expected to display noticeable momentum-dependent nematic features. The effective hopping between *d* orbitals through Bi-*p*x/y orbitals can become nematic once the degeneracy of the *p*x/y orbitals is lifted. Importantly, a strong *d*-*p* hybridization can make the Ti-3*d* orbitals more extended, and thereby enhance the non-local Coulomb interaction, which can promote the nematic bond order.

Thus, the findings by the team would provide valuable insights into the understanding of nematic orders that present in correlated systems and most probably compete with superconductivity.

Contact:
Prof. GAO Hongjun
Institute of Physics, Chinese Academy of Sciences
Email: hjgao@iphy.ac.cn

(IOP)