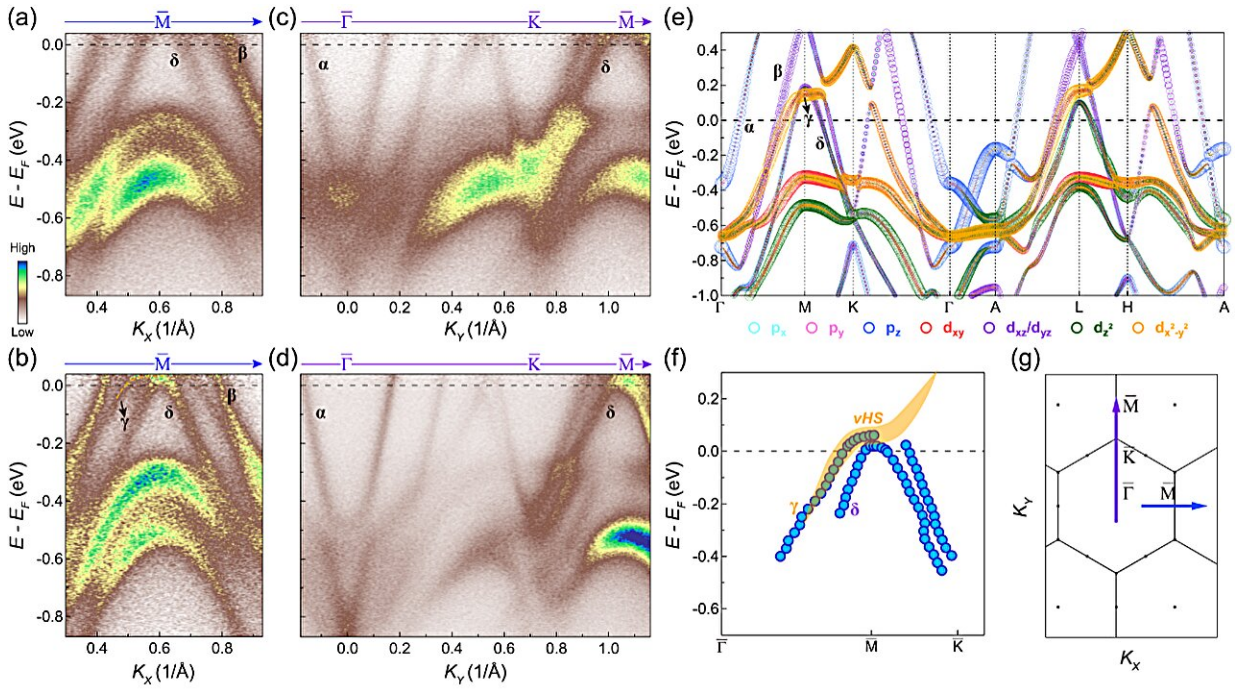
Study discovers tunable van Hove singularity without structural instability

August 22 2023



Evolution of $CsTi_3Bi_5$ electronic structure with Cs doping. Credit: *Physical Review Letters* (2023). DOI: 10.1103/PhysRevLett.131.026701

A team led by Prof. He Junfeng from University of Science and Technology of China (USTC) of the Chinese Academy of Sciences (CAS), together with domestic and international collaborators, discovered that the energy level of the van Hove singularity (VHS) in the novel Ti-based kagome metal $CsTi_3Bi_5$ can be tuned without lattice

structural instability. Their work was published in *Physical Review Letters* on July 12 as the cover article.

In kagome metal, the electronic instabilities provided by VHS usually coexist with lattice structural instabilities, making it difficult to distinguish the effect of different instabilities on charge density waves (CDW).

To understand the effect of different instabilities on CDW, the team conducted research on the novel Ti-based kagome metal $CsTi_3Bi_5$. $CsTi_3Bi_5$ has the same lattice structure as AV_3Sb_5 (A=K, Rb, Cs) but does not have charge density wave states.

The team first studied the electronic structure of $CsTi_3Bi_5$ using high-resolution angle-resolved photoemission spectroscopy and found it in good agreement with the results of first-principles calculations. The energy position of the VHS in pristine $CsTi_3Bi_5$ was well above the Fermi level and cannot bring about electronic instability. First-principles calculations and low-temperature X-ray diffraction measurements showed no lattice instability in $CsTi_3Bi_5$.

Researchers went on to find that electrons can be introduced by Cs surface doping, enabling the modulation of the VHS in $CsTi_3Bi_5$ in a wide energy range. When the VHS approaches Fermi level, it can generate electronic instabilities. At the same time, first-principles calculations showed no lattice structural instability in $CsTi_3Bi_5$ after electron doping. In this way, the team realized the decoupling of the two instabilities. $CsTi_3Bi_5$ can be a unique platform where the electronic instabilities can be modulated solely without being affected by the structural instabilities.

The researchers also found that even if the VHS is tuned to introduce electronic instability near the Fermi energy level, it still can't generate

the energy gap in CDW in $CsTi_3Bi_5$. Thus, the electronic instability itself can't generate charge density waves in $CsTi_3Bi_5$.

First-principles calculations further showed that during the evolution from CsV_3Sb_5 to $CsTi_3Bi_5$, the appearance of CDW directly corresponds to the change in the total energy of the system. CDW phase transition occurs only when the corresponding crystal structure has the lowest total energy. Therefore, lattice structural instability plays an important role in CDW phase transition in kagome metals.

This work is instructive for the further understanding of the effects of electronic instability and lattice structural instability on CDW in kagome metals.

More information: Bo Liu et al, Tunable Van Hove Singularity without Structural Instability in Kagome Metal CsTi3Bi5, *Physical Review Letters* (2023). DOI: 10.1103/PhysRevLett.131.026701

Provided by University of Science and Technology of China