Researchers reveal van Hove singularity at Fermi level in kagome superconductor

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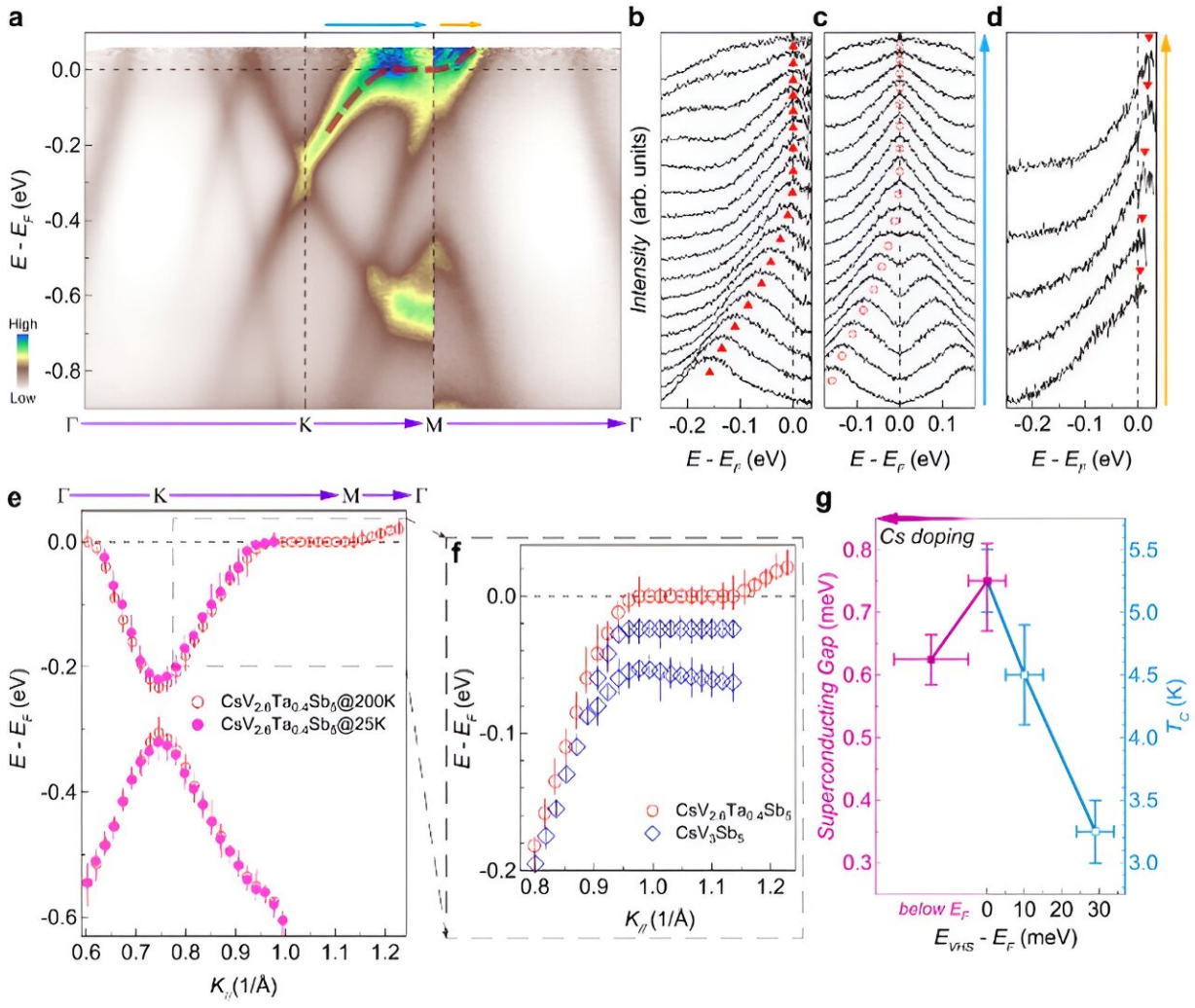

The existence of VHS perfectly aligned with the Fermi level in $CsV_{2.6}Ta_{0.4}Sb_5$. **a** Photoelectron intensity plot along Γ-K-M-Γ of $CsV_{2.6}Ta_{0.4}Sb_5$ measured with 21.2 eV photons at 200 K. This photon energy probes the electronic structure in

the Γ-K-M plane of the 3D BZ . The red dashed lines are a guide for the eye. **b** EDCs near M point extracted from the photoemission raw spectrum in the momentum region marked by the blue arrow in (**a**). **c** Same as the raw EDCs in (**b**), but symmetrized to show the absence of an energy gap. **d** EDCs near M point extracted from the photoemission raw spectrum in the momentum region marked by the yellow arrow in (**a**). The red triangles and circles in (**b**), (**d**) indicate the EDC peaks. **e** Band dispersion near K and M points (along the Γ-K-M-Γ direction) extracted from the EDC peaks measured at 200 K (red empty circles) and 25 K (magenta solid circles), respectively. **f** Extracted band dispersion of $CsV_{2.6}Ta_{0.4}Sb_5$ and CsV_3Sb_5 in the momentum region near M, indicated by the black dotted box in (**e**). The error bars in (**e**) and (**f**) represent the uncertainties in the determination of EDC peak positions. **g** Superconducting T_c (right axis) and superconducting gap (left axis) as a function of the energy position of the VHS in doped CsV_3Sb_5 samples . The error bars in (**g**) represent the uncertainties in the determination of the VHS (bottom axis), superconducting T_c (right axis), and superconducting gap (left axis). Credit: *Nature Communications* (2023). DOI: 10.1038/s41467-023-39500-7

A team led by Prof. He Junfeng from University of Science and Technology of China (USTC) of the Chinese Academy of Sciences (CAS), in collaboration with Academician Gao Hongjun's team from CAS and other domestic and international research teams, has discovered the van Hove singularity (VHS) at Fermi level in kagome superconductors and revealed its relationship with superconductivity. Their work was published in *Nature Communications* on June 28.

VHS is a saddle point connecting electron-like and hole-like energy bands that can generate divergent electron density of states. On the one hand, the luge electron density of states near VHS can cause strong instability in the electronic structure. On the other hand, hole-like and electron-like conduction can coexist at VHS, giving rise to unconventional electronic pairing.

However, in reality, VHS tends to deviate from the Fermi level of the material, resulting in very little effect on the low-energy states of the material. Therefore, it is important to find the suitable kagome material to explore the effect of VHS on superconductivity.

The researchers investigated Ta-doped CsV_3Sb_5 samples, and the use of Ta atoms instead of V atoms can increase the superconducting transition temperature from 2.5 K in CsV_3Sb_5 to 5.5 K in $CsV_{3-x}Ta_xSb_5$ (x~0.4). Angle-resolved photoemission spectroscopy was used to investigate the electronic structures of both CsV_3Sb_5 and Ta-doped $CsV_{3-x}Ta_xSb_5$ samples.

The results showed that the VHS in CsV_3Sb_5 lies below the Fermi level before entering the superconducting state due to the reconfiguration of energy bands by the electron density wave and contributes almost nothing to superconductivity, whereas in $CsV_{3-x}Ta_xSb_5$, the VHS is located exactly at the Fermi level, in agreement with first-principles calculations.

Further experiments demonstrated that there is a strong correlation between the superconducting transition temperature and the energy position of the VHS relative to the Fermi energy level, revealing the feasibility of VHS-enhanced superconductivity in kagome superconductors.

In addition, the researchers found that the superconducting state in $CsV_{3-x}Ta_xSb_5$ has significantly different characteristics from the superconducting state in CsV_3Sb_5 through scanning tunneling microscopy experiments, indicating the possibility of unconventional pairing superconductivity in the van Hove scenario.

More information: Yang Luo et al, A unique van Hove singularity in kagome superconductor CsV3-xTaxSb5 with enhanced

superconductivity, *Nature Communications* (2023). DOI: 10.1038/s41467-023-39500-7