135-kagome metals under pressure: Dimensionality crossover and Fermi surface reconstructions

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Abstract

Kagome metals provide a unique platform where nontrivial band topology (Dirac crossings, flat bands, and van Hove singularities) give rise to density-wave order and superconductivity [1,2]. The strong tunability of these electronic states by external parameters opens new perspectives to explore correlated and topological quantum phenomena. In this talk, I will compare the pressure evolution of three isostructural kagome metals, CsV_3Sb_5, $CsCr_3Sb_5$, and $CsTi_3Bi_5$, combining high-pressure single-crystal X-ray diffraction (XRD) with density functional theory calculations to establish a direct link between lattice evolution and electronic structure.

Despite sharing the same crystal structure, these compounds exhibit very different electronic behaviors that manifest distinctly under pressure. Transport studies reveal rich temperature–pressure phase diagrams. In CsV_3Sb_5, van Hove singularities near the Fermi energy drive a charge-density-wave (CDW) instability coexisting with superconductivity at ambient pressure. Upon compression, suppression of the CDW gives rise to a superconducting dome, followed by a reentrant superconducting phase at higher pressures, forming a characteristic double-dome structure [3]. In contrast, $CsTi_3Bi_5$ lacks both CDW and superconductivity at ambient pressure due to van Hove singularities being located well above the Fermi level; nevertheless, superconductivity emerges under pressure with a similar double-dome profile [4]. In the case of $CsCr_3Sb_5$, flat bands lie closer to the Fermi level, stabilizing a density-wave state at ambient pressure, while superconductivity only appears above ~3 GPa and peaks near 5 GPa [5].

Our high-pressure single-crystal XRD measurements, performed up to 20–25 GPa, reveal a universal yet anisotropic lattice response across all three systems. Owing to the 2D nature of these materials, compression along the *c*-axis is significantly stronger than within the kagome planes. This anisotropic compression drives a pressure-induced dimensional crossover, occurring near ~5 GPa for CsV_3Sb_5 and $CsCr_3Sb_5$, and at a lower pressure of ~3 GPa for $CsTi_3Bi_5$. Concomitantly, we observe a systematic evolution in in-plane stiffness, increasing from CsV_3Sb_5 to $CsCr_3Sb_5$ to $CsTi_3Bi_5$, indicating progressively stronger kagome-plane bonding. In contrast, the *c*-axis compressibility is reduced in $CsTi_3Bi_5$, resulting in a lower overall compressibility anisotropy.

Combined with our previous spectroscopic results on CsV_3Sb_5 [6,7], these findings suggest that pressure-induced interlayer bonding shifts the Sb/Bi *p*-states toward higher energies. This leads to a reconstruction of the Fermi surface and provides a unifying mechanism for the emergence and reentrance of superconductivity. Our results highlight the central role of lattice-controlled dimensional crossover in tuning electronic topology and superconducting instabilities in kagome metals.

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[7] M. Wenzel et al. Phys. Rev. B 105, 245123 (2022)