Supplementary information

Strain-induced quantum phase transition in C₃Sc₄ monolayer:

Towards to multiple gapless fermions

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Strained	<i>C</i> ₁₁ (N/m)	<i>C</i> ₁₂ (N/m)	C ₂₂ (N/m)	C ₄₄ (N/m)
0%	150.122	53.251	150.562	53.217
9.5%	110.334	38.301	110.737	37.099
13%	61.125	25.546	60.696	15.865

Table S1. obtained C_{11} , C_{12} , C_{22} , and C_{44} for C₃Sc₄ at 0 %, 9.5 %, 13 % biaxial strains

In Figure S1, we plot the in-plane Young's modulus, Y, and Poisson's ration, ν , along an arbitrary direction specified with the polar angle θ (θ is the angle relative to *a* direction) can be obtained as below^{S1}:

$$Y(\theta) = \frac{\Delta}{c_{11}s^4 + c_{22}c^4 + (\frac{\Delta}{c_{44}} - 2c_{12})c^2s^2} \quad \text{Eq (S1)}$$
$$v(\theta) = \frac{(c_{11} + c_{22} - \frac{\Delta}{c_{44}})c^2s^2 - c_{12}(c^4 + s^4)}{c_{11}s^4 + c_{22}c^4 + (\frac{\Delta}{c_{44}} - 2c_{12})c^2s^2} \quad \text{Eq (S2)}$$

where $\Delta = C_{11}C_{12} - C_{12}^2$, $c = \cos(\theta)$, and $s = \sin(\theta)$. Using Eqs. (S1) and (S2), and the elastic constants presented in Table S1, the θ dependence of Y and ν on C₃Sc₄ at 0%, 9.5%, 13% biaxial strains are shown with polar coordinates in Figure S1. In such a plot, a fully isotropic elastic behavior is represented by a perfectly circular shape for Y and ν . On the contrary, the shapes of Y and ν in Figure S1 are anisotropic, with major axis and minor axis difference for C₃Sc₄ at 0%, 9.5%, 13% biaxial strains, indicating that the mechanical properties of C₃Sc₄ at 0%, 9.5%, 13% biaxial strains exhibit anisotropy.



Figure S1. The θ dependence of (a) Y and (b) ν for C3Sc4 at 0% (left), 9.5% (middle), 13% (right) biaxial strains.

Reference

(S1) E. Cadelano, P. L. Palla, S. Giordano and L. Colombo, Phys. Rev. B: Condens. Matter Mater. Phys., 2010, 82, 235414.