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High-entropy engineering of the crystal and electronic structures in a Dirac material

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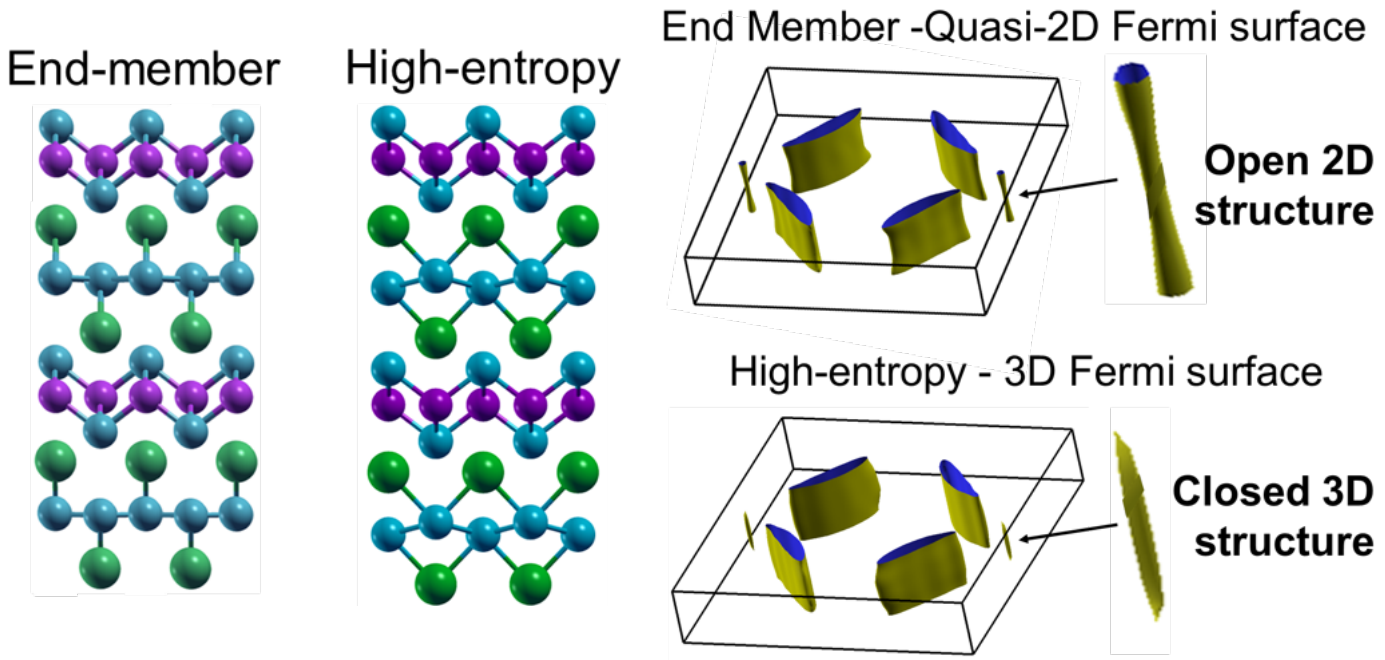
Quantum materials have the potential to revolutionize technologies ranging from sensing to telecommunication and computation. However, advancement has been limited by the development of topological and Dirac materials. IRG2 researchers demonstrated a novel and widely applicable strategy to engineer relativistic electron states to develop such materials through a high-entropy approach.

The Dirac states of single crystalline (Ca,Sr,Ba,Eu.Yb)$MnSb_2$ Dirac semimetal were found to differ in character from those of its end-members. While the end-member compositions host quasi-2D Fermi surfaces, that of the high-entropy phase is quasi-3D. The sharing of the high-entropy sublattice by multiple species distorts the crystal structure locally, giving rise to a 3D Fermi surface.

Shubnikov–de Haas oscillations measurements were performed to determine the aspect ratio of the Fermi pocket. First-principles calculations validated these measurements and supported the proposed mechanism underpinning the engineering of the electronic structure.



Left: Diagram of the undistorted crystal structure typical of the end members and the distorted structure of the high entropy phase. Note the corrugation of the Sb layers (blue).

Right: Fermi surface of the undistorted end members and the distorted high entropy structure. Note the formation of a closed Fermi pocket in the latter.