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Tuning surface Dirac valleys by strain in topological crystalline insulators IJIANFENG WANG, Beijing Computational Science Research Center, LU ZHAO, Beihang University, BING-LIN GU, WENHUI DUAN, Tsinghua University — Topological crystalline insulator has an even number of Dirac cones (i.e., multiple valleys) in its surface band structure, thus potentially leading to valleytronic applications such as graphene. Using the density-functional-theory method, we systematically investigate the strain-induced evolution of topological surface states on the SnTe(111) surface. Our results show that compressive strain can shift the Dirac cones at the $\bar{\Gamma}$ and \bar{M} valleys to different extents (even oppositely) in energy, while tensile strain can induce different band gaps at the valleys due to the enhanced penetration depths of surface states. Exploiting a strain-induced nanostructure with well-defined edges on the (111) surface, we demonstrate strong valley-selective filtering for massless Dirac fermions by dynamically applying local external pressure. Our findings may pave the way for strain-engineered valley-resolved manipulation of Dirac fermions with high tunability and scalability.

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