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Electronic structure and topological transition of SnTe at high pressure[1] QUAN LI, DAN ZHOU, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA, YANMING MA, State key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA — Recent x-ray diffraction measurements and first-principles calculations have revealed intriguing structural evolution of tin telluride (SnTe) under high pressure. Here we report on a systematic study of the electronic band structure, density of states, Fermi surface and charge density of SnTe at high pressure using first-principles density functional theory calculations. Our results unveil an electronic topological transition in the cubic Fm-3m phase of SnTe with its Fermi surface changing from disconnected pockets to inter-connected quasicubic tubes near the L points of the Brillouin zone under high pressure. The pressure-induced quasicubic tubular Fermi surface is similar to that previously obtained via carrier doping. The induced change in electronic charge distribution stabilizes the Fm-3m structure and thus suppresses the transition to the rhombohedral structure, which explains experimental observations. Furthermore, our calculations show that pressure-induced electronic topological transition is also present in the orthorhombic Cmcm and Pnma phases of SnTe in the pressure range of 5 to 18 GPa, but this transition is absent in the high-pressure (above 18 GPa) Pm-3m phase.

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