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Unraveling Convoluted Structural and Electronic Transitions in SnTe at High Pressure[1] DAN ZHOU, QUAN LI, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA, YANMING MA, QILIANG CUI, 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 — The longstanding uncertainty in high-pressure structural evolution of SnTe has greatly impeded the understanding of its complex electronic properties. Here we unravel the convoluted high-pressure phase transitions of SnTe using angle-dispersive synchrotron x-ray diffraction combined with first-principles structural search. We identify three coexisting intermediate phases of Pnma, Cmcm, and GeS type structure and establish the corresponding phase boundaries. We further unveil the intricate pressure-driven evolution of the energetics, kinetics and lattice dynamics of SnTe to elucidate its distinct phase-transition mechanisms. Subsequent electronic band calculations reveal pressure-induced metallization, superconductivity and topological phase transition in SnTe. These findings resolve structures and predict intriguing properties of SnTe, which have broad implications for other IV-VI semiconductors that likely harbor similar novel high-pressure phases and properties.

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