High Pressure Study on Novel Quantum Materials

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Pressure provides a useful tool to precisely tune the interatomic distances in quantum materials, which is critical to understanding the organizing principles that govern electron dynamics with strong quantum fluctuations. Here, we report a comprehensive high-pressure study on the layered antiferromagnetic CaMn2Bi2 and discovered that it undergoes a pressure-induced structural phase transition with a large volume collapse $\Delta V/V \sim 10\%$ at about 3 GPa. The crystal structure of the high-phase phase shows CaMn2Bi2 crystallizes in a new monoclinic structure with space group P21/m, and the puckered Mn-Mn honeycomb lattice in the ambient-pressure phase is found to be converted to one-dimensional (1D) zigzag ladder-like chains in the high-pressure phase. High-pressure resistivity measurements also evidenced the structural transformation as a sudden drop of resistivity by nearly two orders of magnitude at Pc = 2.4 GPa. In contrast to the semiconducting behavior at low temperatures of the low-pressure phase, the high-pressure monoclinic phase at P > Pc exhibits a metallic behavior down to the lowest temperature and displays in the resistivity curves two characteristic anomalies which show opposite pressure dependences. Considering the quasi-1D characteristics and enhanced electrical conductivity in the high-pressure phase, these anomalies might be associated with the formation of some spin/charge-density-wave states. The second electronic phase may result from the instability of the Fermi surface and strong electron-phonon coupling in the quasi-1D Mn-Mn chains. The theoretical assessments of electronic structures and total energies calculated for various magnetic structures of monoclinic CaMn2Bi2 indicate that the ferrimagnetic magnetic pattern is favored thermodynamically.