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Dirac semimetal phase in the hexagonal LiZnBi WENDONG CAO, Department of Physics, Tsinghua University, Beijing 100084, China, PEIZHE TANG, Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA, YONG XU, Department of Physics, Tsinghua University, Beijing 100084, China, JIAN WU, Department of Physics, Tsinghua University, Beijing, BING-LIN GU, Institute for Advanced Study, Tsinghua University, Beijing 100084, China, WENHUI DUAN, Department of Physics, Tsinghua University, Beijing 100084, China — Based on first-principles calculations, we find that LiZnBi, a metallic hexagonal ABC compound, can be driven into a topologically nontrivial Dirac semimetal by strain. The nontrivial topological nature of the strained LiZnBi is directly demonstrated by calculating its Z_2 index at $k_z = 0$. We show that there are two Dirac points located at the rotation axis, protected by C_{6v} symmetry and time-reversal symmetry. In the calculated surface states, the Fermi arcs connecting the projections of these two Dirac points are found. We also present how the low-energy states as well as topological properties change under different strain configurations. The finding of Dirac semimetal phase in LiZnBi may intrigue further researches on the topological properties of hexagonal ABC materials and promote new practical applications.

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