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Topological phase transitions in $TlBiS_2$ and $TlSbS_2$ under strain

QINGYUN ZHANG, YINGCHUN CHENG, UDO SCHWINGENSCHLOGL, Physical Sciences and Engineering, King Abdullah University of Science and Technology, COMPUTATIONAL PHYSICS AND MATERIALS SCIENCE TEAM — Using first-principles calculations, we investigate the band structure evolution and topological phase transitions in $TlBiS_2$ and $TlSbS_2$ under hydrostatic pressure as well as uniaxial and biaxial strain. For $TlBiS_2$ topological transitions occur around 0 and 5 GPa, the system remaining a direct gap semiconductor up to 8 GPa. On the other hand, for $TlSbS_2$ the transitions occur around 2 and 5 GPa and the system transform from a direct gap semiconductor to a semimetal around 2 GPa. Biaxial and uniaxial strains are compared to each other. The phase transitions are identified by parity analysis and by calculating the surface states. Zero, one and four Dirac cones are found for the (111) surfaces of both $TlBiS_2$ and $TlSbS_2$ when increasing the pressure, which confirms the trivial-nontrivial-trivial phase transitions. The Dirac cones at the M points are anisotropic with a large out-of-plane component and inversely related in-plane spin and momentum direction. By examining the states on different surfaces we show that $TlBiS_2$ under 8 GPa pressure is a topological crystalline insulator. This finding makes the thallium-based III-V-VI2 ternary chalcogenides candidates for studies on topological crystalline phase.

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