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Strain-induced topological phase transitions in HgTe¹ NIRPEN-DRA SINGH, Material Science and Engineering Division, KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia, RAVINDRA PANDEY, Department of Physics, Michigan Technological University, Houghton, MI 49931, USA, AMBESH DIXIT, Indian Institute of Technology Jodhpur — Mercury telluride is a known semi-metal in its bulk zinc-blende structure with electronic bandgap $E_g \sim -0.3$ eV and has been predicted to be a topological insulator under strain. In this study, we carried out ab initio electronic structure calculations to investigate the transition of HgTe system from semi-metal into the topological insulating phase under compressive strain along [001], [110] and [111] directions. The compressive strains along these directions close and reopen a gap at the Γ point and topological phase is emerged. We will discuss the evolution of topological insulator phase in the context of semimetal nature of bulk HgTe system.

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