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Prediction of Robust Non-centrosymmetric Topological Dirac Semi-metallic State in Ternary Half-Heusler Compounds KOUSHIK PAL, UMESH WAGHMARE, Jawaharlal Nehru Ctr Adv Sci, MATERIALS THEORY GROUP TEAM — Topological Dirac semi-metal (TDSM), a novel quantum state of matter with exotic transport, magnetic, chiral and superconducting properties, has been a subject of intense research in recent years. TDSM is a 3-dimensional analogue of graphene, and is also interesting as a parent to other topological states. Although half-Heusler (HH) compounds were shown to exhibit rich topological phases, a robust TDSM phase in them is yet to be discovered. Here, we present a generic topological phase diagram of a large family of HH compounds with strained structures maintaining a three-fold symmetry, and discover their highly robust non-centrosymmetric TDSM state. We show that its symmetry permits a direct control of valley current with parallel electric field. Using an existing, stable half-Heusler LiMgBi as a model system in first-principles theoretical analysis we show that topological semi-metal, topological Dirac semi-metal, normal and topological insulating states are common to strained structure of these HHs which can be realized experimentally through epitaxially grown hetero-structures. Uncovering many HHs exhibiting a variety of topological states, our work opens up exciting phenomena involving chirality, polarity, valley and topology that have the potential for novel technologies.

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