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Topological crystalline insulator states in layered materials YOUNGKUK KIM, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, CHARLES KANE, EUGENE MELE, Department of Physics and Astronomy, University of Pennsylvania, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — Topological crystalline insulator (TCI) is a topological state of materials whose topological property relies on generic crystalline symmetries. Based on firstprinciples calculations, we suggest new classes of topological crystalline insulators characterized by non-zero mirror Chern numbers (MCNs) hosted on the mirrorinvariant plane at the boundary of the Brillouin zone (BZ). We demonstrate that the new TCI phases can be realized in layered materials, and the topological phase transitions associated with the proposed TCI phases occur under an external pressure. Our results shed light on the role of the MCNs hosted on the surface of the BZ, and open new possibilities for finding TCI materials.

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