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Effects of edge terminations on monolayer topological crystalline insulators via group theory and DFT[1] GERSON J. FERREIRA, AUGUSTO L. ARAUJO, Federal University of Uberlandia, ERNESTO O. WRASSE, Universidade Tecnologica Federal do Parana, TOME M. SCHMIDT, Federal University of Uberlandia — Topological crystalline insulators (TCIs) are a counterpart of usual topological insulators in materials where the topological edge (or surface) states are protected by the underlying crystal symmetries. Here we discuss the band structure of IV-VI monolayer materials, where the edge states are protected by mirror symmetry, considering ribbons cutted in different orientations and distinct edge terminations. We show that although the Chern numbers and the topological classification remain a bulk property, the nature of edge terminations and orientation play a significant role in TCIs. For each ribbon an effective Hamiltonian is derived by group theory and proper boundary conditions are presented. These show good agreement with DFT calculations and illustrate the effects of the distinct reduced symmetry of each ribbon type.

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Gerson J. Ferreira
Federal University of Uberlandia

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