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Electronic and spin structure of topological surface state in Sn-based ternary topological insulators MAIA G. VERGNIORY, Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain, TATIANA V. MENSHCHIKOVA, Tomsk State University, pr. Lenina 36, Tomsk, 634050 Russia, IGOR V. SILKIN, Tomsk State University, Tomsk, 634050 Russia, YURY M. KOROTEEV, SERGEY V. EREMEEV, Institute of Strength Physics and Materials Science, Siberian Branch, Russian Academy of Sciences, Tomsk, 634021 Russia, EVGUENI V. CHULKOV, Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain, CHULKOV GROUP TEAM — We report the bulk and surface electronic properties and spin polarization of a new rich family of Sn-based ternary complex topological insulators studied by means of first principles calculations. These compounds exist in different stoichiometries: SnxAyBz (A:Sb and Bi) (B: Te and Se). The crystal structure of these compounds are characterized by alternating along hexagonal axis quintuple, septuple and nonuple layer van der Waals bonded building blocks. We reveal that the bulk band gap in these systems is about 200 meV and the spin polarization near the Dirac point is up to 85%, one of the highest predicted hitherto. At the same family, for some of these compounds which crystal structure has ionic-covalent bonded Bi2Te3 and crystalline topological insulator SnTe atomic layers within building block the complex SOI-induced bulk band inversion caused by competition of band inversions in Bi2Te3 and in SnTe layers occurs and results in inherently nonlinear dispersion of the topological surface state.

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