Electronic properties of bismuth and antimony thin films

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In the following work topological properties of bismuth and antimony thin films are investigated using density functional theory and tight-binding method. Bismuth bilayer was among first 2-dimensionals systems predicted to exhibit quantum spin Hall effect [1]. Several experiments have confirmed topological nature of edge states in Bi [2], although there is still on-going debate how robust this effect is with respect to number of layers and type of substrate [3]. Contrary to bismuth, free-standing antimony bilayer is known to be trivial semiconductor [4]. When increasing thickness of this material, it undergoes topological phase transition to 2D QSH phase, then to 3D topological insulator and finally to topological semimetal. Phase diagram of this material can be significantly modified by application of strain and electric fields [5], e.g. for sufficient tensile strain turning bilayer Sb to topological insulator.

Motivated by those studies, we investigate topological properties of thin Bi and Sb films. First, electronic structures of Bi and Sb are calculated using density functional theory. Then, sp^3 tight-binding model [6] is fitted to our dft results, paying special attention to band structure around band-gap region and orbital compositions of conduction and valence bands for both Bi and Sb. In next step, Bi-Bi, Sb-Sb structures and Bi-Sb heterostructure are studied. By careful investigation of separated Bi and Sb electronic structure and then effect of their interaction, we extract tight-binding parameters describing interlayer interactions in all systems. Then the effects of spin-orbit coupling strength and interlayer interaction strength on Z_2 invariant and spin textures are presented. Topological nature of edge states in this system is probed in the nanoribbon geometry for both zigzag and armchair edge types.

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