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First-principles study of topological surface states in Bi_2Se_3/ZnSe superlattices[1] KYUNGWHA PARK, Virginia Tech, Blacksburg, ZHIYI CHEN, LUKAS ZHAO, THOR AXTMANN GARCIA, MARIA TAMARGO, LIA KRUSIN-ELBAUM, The City College of New York, CUNY — Topological insulators (TIs) are interesting due to robustness of surface states within a bulk band gap in the presence of time reversal symmetry. Various TI heterostructures are based on the robustness of the topological surface states. Thus, it is crucial to understand how the topological surface states are influenced by interfaces. Recently $Bi_2Se_3/Zn_xCd_{1-x}Se$ superlattices grown by molecular beam epitaxy showed interesting magneto-transport properties such as a single two-dimensional conducting channel per TI layer with the Berry phase of π. Intrigued by this experiment, we investigate topological surface states of the Bi_2Se_3/ZnSe superlattice by using density-functional theory. Based on the stoichiometry and the charge balance of the ZnSe layer, when one side of the ZnSe layer is terminated with Zn in the superlattice, the other side must be terminated with Se. Using the superlattice model and two slab models with either a Zn-terminated or Se-terminated interface, we calculate the effect of the inherent asymmetry of the ZnSe layer on the topological surface states of Bi_2Se_3, and compare our result to the experiment.

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