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Ab initio study of topological insulating property in the heterojunction of Bi (111) bilayer and Bi_2Te_2Se KYUNG-HWAN JIN, SEUNG-HOON JHI, Department of Physics, POSTECH — Study of topological insulator (TI) is showing rapid progress in both theory and experiment, particularly on three dimensional materials. Examples of two dimensional TI (quantum spin Hall) materials are, on the other hand, comparatively less common. As such, theoretical predictions of single Bi (111) bilayers as TI draw great attention from experiment. A recent report of ARPES measurements claims verification of the 2D TI property of Bi bilayer, but analysis leaves much room for further clarification. Because Bi (111) bilayers grown on 3D TI substrates such as Bi_2Te_3 and Bi_2Te_2Se; understanding the details of the interface between the Bi bilayer and 3D TI substrates is essentially required. We study the electronic structures of Bi bilayer-Bi_2Te_2Se heterojunction from first-principles calculations. We find a substantial shift of Dirac cone from the TI substrates into Bi bilayer that thus becomes metallic on TI substrates. It is shown that the origin of this change is the inversion-symmetry breaking in Bi bilayer due to TI substrate. By comparing our calculations of Bi bilayer nanoribbons on Bi_2Te_2Se with STM/STS measurements, we successfully resolve and locate the edge states of a single Bi bilayer and confirm its 2D TI character.

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