

Abstract Submitted
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Band alignment and bending in Dirac semimetal Na₃Bi thin films on Al₂O₃ substrates¹ KYUNGWHA PARK, JOHN VILLANOVA, Virginia Tech — Dirac semimetals Na₃Bi and Cd₃As₂ are interesting due to topologically protected degenerate Weyl nodes with linear dispersions at the Fermi level and topological Fermi-arc surface states. Recently, thin films of Na₃Bi have been epitaxially grown on Al₂O₃ substrates and their electron transport properties have been measured. However, the interfaces between the Dirac semimetal films and the substrates have not been characterized yet. Here we investigate electronic and topological properties of thin Na₃Bi films on Al₂O₃ substrates near the Fermi level, by using density-functional theory with spin-orbit coupling. We also discuss effects of band alignment and band bending on the electronic and topological properties and compare with experimental data.

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