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Electronic structure study of Topological Insulator Bi_2Se_3 on graphene substrates[1] XUEPING JIANG, Rensselaer Polytechnic Institute, BHANU MAHANTI, Michigan State University, SAROJ NAYAK, Rensselaer Polytechnic Institute, Indian Institute of Technology Bhubaneswar, RENSSELAER POLYTECHNIC INSTITUTE COLLABORATION, MICHIGAN STATE UNIVERSITY COLLABORATION, INDIAN INSTITUTE OF TECHNOLOGY BHUBANESWAR COLLABORATION — In recent experiments, graphene has been found to be a suitable substrate for Topological Insulators (TIs) due to better lattice match and smaller defect density. Recent studies have also shown that the presence of a substrate can modulate the electronic properties of TIs. One system that has not been well studied is Bi2Se3 supported by graphene. In this work, density functional theory has been used to study the electronic structure of such a heterostructure. Six quintuple layers (QLs) and one QL were considered for Bi2Se3. When six QLs of Bi2Se3 are supported by graphene on either one or both sides, the Dirac cone of the TI is shifted below the Fermi energy and a band gap is opened in graphene. In addition, the influence of the graphene substrate on the topological surfaces states is negligible. The four-fold degeneracy around the Dirac point for Bi2Se3 is maintained when the TI is supported on both sides by graphene, but is split when graphene is deposited on only one side. For one QL Bi2Se3 the electronic structure near the band gap was strongly perturbed due to the interaction with graphene orbitals. These results will be compared with other works of TIs on substrates.

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