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Ab initio study of adatom adsorption on topological insulator thin film KYUNG-HWAN JIN, Department of Physics, Pohang University of Science and Technology, SEUNG-HOON JHI, Department of Physics and Division of Advanced Materials Science, Pohang University of Science and Technology —
Recently topological insulator has attracted great attention due to its intriguing electronic and transport properties. Topological insulator has bulk energy gap but conducting surface states which are chiral with a linear energy-momentum relation. These surface states are robust against external perturbations as they are protected by the time reversal symmetry. We studied the electronic structure of topological insulator Bi_2Te_3 thin film and investigated how it is modified upon the adsorption of single atomic impurities using first-principles calculations. We chose nitrogen (N), oxygen (O), sodium (Na) and cobalt (Co) atoms to study their adsorption on top of Bi_2Te_3surface. We investigated the effect of non-magnetic and magnetic impurities on the surface states, and the band splitting due to the inversion symmetry-breaking by the Rashba field.

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