

Magnetic properties of Gadolinium doped Bismuth Tellurides: First-principles calculation

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Due to the strong localized f states of the rare-earth elements, the Bi₂Te₃based alloys with rare-earth dopings have been found to show various magnetic and transport phases and interesting phase transitions [1]. In this report, we studied the magnetic and electronic structures of the gadolinium doped Bi₂Te₃ with different doping sites in order to investigate the magnetic phase stability and its dependence on the doping site by first-principles calculation within DFT, employing the precise full-potential linearized augmented plane-wave (FLAPW) method [2]. The spin-orbit coupling interaction and the strong correlation effect are included by the second variational method and +U corrections, respectively. The total energy comparison for the uniform and the clustering type distributions for various magnetic phases and their band structures will be discussed. Also the formation energy calculations will reveal the preference Gd substitution sites into the tellurides.

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