Impact of Vanadium Doping on Magnetic Properties and Curie Temperature of HgTe: Heisenberg model and GGA study

mohamed baiboud[1]

[1] *LMS3E*

The ab-initio study was performed using the genaralized Gradient Approximations (GGA) implemented in the CASTEP code to investigate the impact of vanadium doping on the electronic, optical, and magnetic properties of HgTe. The calculated lattice parameters of the compound under ambient conditions showed good agreement with experimental data. The pure HgTe compound is a semimetal, with the higher energy states of the valence band only overlapping the lower energy states of the conduction band. Doping with vanadium (V) induces ferromagnetism in the system, leading to a significant spin polarization of about 90% at the Fermi surface, making HgTe a potential candidate for spintronic applications. The Curie temperature (TC) was estimated using mean field theory for doping concentrations of 12% and 24%. The double exchange is suggested as the most responsible interaction of ferromagnetism in the system. Optical calculations indicate enhanced absorption in the visible and infrared regions, suggesting its viability for optoelectronic device applications. These findings pave the way for the design of transition metal-doped HgTe for the technological advancement of spintronics and photonics in the future.