



Tuning the structural stability and electronic properties of BiTe nanostructures-a density functional theory study

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Abstract: The realistic nanostructures of pristine, Se and S incorporated BiTe nanostructures in the form of nanocone, nanosheet and nanotube are optimized and simulated successfully using density functional theory along with B3LYP/ LanL2DZ basis set. The formation energy, chemical potential and chemical hardness are used to study the structural stability of BiTe nanostructures. Point symmetry and dipole moment of pristine, Se and S incorporated BiTe nanostructures are also reported. The electronic properties of BiTe nanostructures are discussed in terms of ionization potential, electron affinity and HOMO-LUMO gap. The present work reveals that the incorporation of impurities leads in enhancing the structural stability and electronic properties of BiTe nanostructures, which find its application in power generator and gas sensors.

Keywords: bismuth telluride, nanostructure, formation energy, dipole moment, HOMO-LUMO.

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