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Electronic Structure Calculation of AsSiTeB/SiAsBTe Nanostructures Using Density Functional Theory

Authors : Ankit Kargeti, Ravikant Shrivastav, Tabish Rasheed

Abstract : The electronic structure calculation for the nanoclusters of AsSiTeB/SiAsBTe quaternary semiconductor alloy belonging to the III-V Group elements was performed. Motivation for this research work was to look for accurate electronic and geometric data of small nanoclusters of AsSiTeB/SiAsBTe in the gaseous form. The two clusters, one in the linear form and the other in the bent form, were studied under the framework of Density Functional Theory (DFT) using the B3LYP functional and LANL2DZ basis set with the software packaged Gaussian 16. We have discussed the Optimized Energy, Frontier Orbital Energy Gap in terms of HOMO-LUMO, Dipole Moment, Ionization Potential, Electron Affinity, Binding Energy, Embedding Energy, Density of States (DoS) spectrum for both structures. The important findings of the predicted nanostructures are that these structures have wide band gap energy, where linear structure has band gap energy (Eg) value is 2.375 eV and bent structure (Eg) value is 2.778 eV. Therefore, these structures can be utilized as wide band gap semiconductors. These structures have high electron affinity value of 4.259 eV for the linear structure and electron affinity value of 3.387 eV for the bent structure form. It shows that electron acceptor capability is high for both forms. The widely known application of these compounds is in the light emitting diodes due to their wide band gap nature.

Keywords : density functional theory, DFT, density functional theory, nanostructures, HOMO-LUMO, density of states
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