Investigating the electronic properties of $C_{20-n}Si_n$ and $C_{20-n}Ge_n$ (n=1-5) nano structures using density functional theory

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Abstract

In this research, the thermodynamic stability, energy of gap and electrical conductivity of nano structures of C_{20} bowl, $C_{20-n}Si_n$ (n=1-5) and $C_{20-n}Ge_n$ (n=1-5) were investigated at the level of Quantum calculations of LSDA/6-31G of Density Functional Theory (DFT) at the room temperature. We studied the application of these structures in solar cells. The most stable structures are $C_{15}Ge_5$ and $C_{17}Si_3$ at 300 K. The results show that the substitutes decrease the gap of energy and increase the electrical conductivity, but the number of Silicon or Germanium substitute does not have a regular effect on the gap of energy. The $C_{17}Ge_3$ and $C_{16}Si_4$ have the lowest gap of energy with more conductivity. The gap of HOMO and LUMO energy levels of the electron donor and electron acceptor components is the most important factor for the electron transfer with photovoltaic application potential. The two structures of $C_{17}Si_3$ as electron acceptor and $C_{15}Ge_5$ as electron donor with the maximum voltage of 1.93 volt can be used in producing solar cell.

Keywords: Silicon Substitution, Germanium, Density Functional Theory, Energy Gap, C_{20} Bowl, V_{oc}

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