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Investigation of electron transport properties in Fullerene and Fullerane nanocages

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Abstract

In this research, we investigate the electron transport in fullerene and fullerane nanocages. We study the electron transport of these systems based on the tight-binding model with the approximation of the nearest neighbors and the formulation of the Green's function. In this research, we consider the type of electrodes attached to molecules as cumulene carbon chains, and investigate the effect of the position of the electrodes on the electron conductance of the mentioned nanocages. We obtain the structural properties of the molecules with the help of density functional theory, and the use of the B3LYP hybrid function. We study the electrical conductance of these systems by forming molecular bridges between two cumulene electrodes. To do this, we first obtain the stable states of the connection of the electrodes to the desired systems using the density functional theory. Our results show that by changing the position of the connection of the electrodes to the fullerene cage, the electrical properties of these systems can be controlled to observe the phase transition between semiconducting and metal behavior. Also, due to the localization phenomenon, fulleranes are always insulator.

Keywords: Tight-binding, Density functional theory, Fullerene, Fullerane, Cumulene

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