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The effect of dimerization strength and comb-like bond's hopping energy on electronic conductance and density of states of typical polyacetylene polymers

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Abstract

In this paper, we study the electronic conductance and density of states for a comb-like polymer with periodic hopping energies in the tight-binding approach. Electron transmission coefficient and density of states are analytically calculated by using Green's function of the system. The results show that the electronic conductance spectrum has one energy gap in the absence of carbon-hydrogen bond's hopping energy, which is proportional to the dimerization strength. Carbon-Hydrogen bond's hopping energy makes the appearance three energy gaps in the conductance spectrum and the dimerization strength influences only the outer gaps.

Keywords: nanowire, electronic conductance, Green's function, dimerization strength, density of states, polyacetylene

For full article, refer to the Persian section