

Abstract

Present paper deals with the electronic structure of some suggested compounds based on anthracene molecule for photovoltaic applications as dyes sensitized solar cells. The studied compounds were initially designed at the Gauss View 5.0.8 program and then relaxed by performing the B3LYP-DFT hybrid functional together with the 6-31G basis sets at Gaussian 09 package of programs to study and analyze of ground state and spectroscopic properties of the compounds. The DFT method was performed to study of the excited states properties of the studied compounds.

The results showed good relax was obtained for the compounds from the used DFT theoretical method. The calculated values of geometrical parameters and virial ratio of the compounds are in a good agreement with experimental data and other theoretical studies. The total energy is independent on the position of the same subgroup in the compounds, it depends only on the number of electrons in each compound.

From the calculations, the results showed the studied compounds show destabilization of LUMO and stabilization of HOMO, they both changed significantly to suggest different structures play important roles in electronic properties. The effect of symmetry and distribution of aromatic rings has an influence on the calculation of HOMO and LUMO. The results of the energy gap showed the inserting the double and triple carbon-carbon bonds between the backbone anthracene molecule and the phenyl rings in both donor and acceptor sides, and the presence of an electron attracting NO₂ subgroups in the compounds

reducing the band gap of the compound. Thus, increasing the conjugation length of the compounds make the compounds to take place in the charge transfer processing