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A Theoretical Study of Geometry Optimization and Energies for Donor-π bridge-Acceptor Molecular System: B3LYP/DFT Calculations

Ghaleb Al-Dahash[1]*, H.I. Abbood[2], Ghaidaa A. Hafed[2], Basim Abdullattif Ghalib[1]

[1]Department of Laser Physics, College of Science for girls, University of Babylon, Hilla-IRAQ
[2]Department of Physics, College of Science, University of Babylon, Hilla-IRAQ

Abstract : B3LYP/6-31G (d , p) density functional theory has been employed to calculate the geometry optimization and energies of donor- π bridge-acceptor molecular system. The electronic state of the system has been calculated depend on Koopman's theorem under the orbital-vertical theory. The results show that the functional used in the description of the studied molecular system has been proved its validity in calculating the HOMO and LUMO energies and it is a suitable for studying the geometry optimization for the organic molecular system. The energy level diagram shows that there are localized orbitals in different parts of the D-B-A molecular systems in which that satisfy important property for the D-B-A system as a molecular electronics.

Keywords: DFT, Koopmanns theorem, Energy gap, HOMO and LUMO, Molecular System: B3LYP/DFT.

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