THEORETICAL COMPUTATIONAL STUDY OF ELECTRONIC STUCTURE OF AROMATIC AND LINEAR π-CONJUGATE SEMICONDUCTOR

INSTITUT PENGURUSAN PENYELIDIKAN

UNIVERSITI TEKNOLOGI MARA

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PREPARED BY:

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AHMAD NAZIB ALIAS

INTAN SYAFFINAZZILLA ZAINE

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KELULUSAN PERMOHONAN DANA KECEMERLANGAN 06/2010

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Dengan hormatnya perkara di atas adalah dirujuk.

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Sekian, harap maklum.

"SELAMAT MENJALANKAN PENYELIDIKAN DENGAN JAYANYA"

Yang benar

MUSTAFAR KAMAL HAMZAH
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ABSTRACT

Polymer is widely used in electrical and electronic applications. To determine the electronic structure of material is very challenging. Nowadays by using mathematical software and programming, most of material structure can been solved. For polymer, many of theoretical physicist and chemist try to solve the unique properties of electronic structure. Hückel Molecular Orbital (HMO) method had been used to determine the suitable parameter to calculate electronic energy level of aromatic and linear π-conjugate and to calculate the electronic energy level of aromatic and linear π-conjugate semiconductor. The analysis of electrical properties (electrical bandgap) of organic semiconductor based on theoretical result shows that the electrons are distributed in the whole molecule. The resonance integral corresponds to the energy of an electron that is shared by two neighboring sp^2-hybridized carbons. It also describes the strength of the interaction of atomic orbital of different atom pairs in a molecule. Based on the electrochemical data, biphenyl has higher atomic interaction that is 4.97 eV followed by naphthalene; 4.54 eV, phenanthrene; 4.40 eV and anthracene 4.28 eV. We can conclude that, the material with higher band gap has higher interaction between two adjacent atoms. In the conjugated organic semiconductor, carbon has sp^2 or sp hybrid state. The Coulomb and resonance integrals for s_σ, p_σ and p_π were different. We predicted the Fermi Energy level by using Peierls Distortion which was laid between 0.9 eV - 1.1 eV. Monomer is assumed as a unit cell. In our calculation, the monomer assumed that an ideal periodicity in lattice structure. For the HOMO and LUMO level, positive and negative changes in coefficient of LCAO showed the change in wavefunction in every monomer unit.