Organic Semiconductor Characterization Using Linear Combination of Atomic Orbital (LCAO)

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ABSTRACT

The electronic structure of conjugated polymer (π-polymer) is calculated using Linear Combination of Atomic Orbital (LCAO). LCAO is a quantum superposition technique to calculate energy level of molecular orbital (MO). This article discusses the electronic structure of naphthalene and polyacetylene (PA). Naphthalene and its derivative are aromatic molecules that are widely used as a hole transport layer in most organic light emitting diode (OLED) applications. In calculating energy level, the basic electronic molecule frame work and Secular determinant must be determined. The band energy of PA is calculated using Ritz Method where H_{ii} determines the interaction of electrons in an isolated $2p_z$ orbital while S_{ij} measures the overlapping between basis function. In microscopic level, the important parameters are Highest Occupied Molecular Orbital (HOMO) which is equivalent with conduction band and Lowest Unoccupied Molecular Orbital (LUMO) which is equivalent with valence band. For Naphthalene, the positive and negative changing in

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coefficient of LCAO shows the changing in wavefunction in every monomer unit and its effects on the electronic properties. In polyacetylene, Fermi Energy levels lay between -0.9 eV and -1.1eV.

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