ANALISIS TEORETIS ZAT WARNA TIPE D-π-A BERBASIS DIFENILAMIN SEBAGAI SENSITIZER PADA SEL SURYA MENGGUNAKAN METODE *DENSITY FUNCTIONAL THEORY* (DFT)

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ABSTRACT

Theoretical Analysis of Diphenylamine-Based D-π-A Dyes as Dye in Solar Cells Using the *Density Functional Theory* (DFT) Method

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Inorganic dyes were first utilized by DSSC as sensitizers. In contrast, inorganic dyes are toxic and only exist in small amounts. However, compared to inorganic dyes, organic dyes do not provide as high an absorption efficiency. Organic dyes can be modified to be type D-π-A (Donor-π conjugation-Acceptor) dyes in an effort to enhance the effectiveness of sunlight absorption. In this study, diphenylamine was used as the electron donor chain with variations of the conjugated π chain and the acceptor chain. Computational studies in this study were carried out using Gaussian 16W software with the DFT method and TD-DFT (Density Functional Theory/Time Dependant DFT) basis set B3LYP/6-31G. The calculation parameters used to determine the efficiency of DSSC as a sentitizer are the bandgap value, absorption wavelength of sunlight, ΔG^{inj}, ΔG^{reg}, oscillator strenght, dihedral angle, bond length, dipole moment, LHE (Light Harvesting Efficiency) and V_{oc} (open-circuit voltage). The results showed that DAPhiA5 dye has the most potential to be used as a sensitizer in DSSC with a bandgap value of 1.7252 eV, wavelength 1090.15 nm, ΔG^{inj} -1.8753 eV, ΔG^{reg} 0.5293 eV, and V_{oc} 0.3859 eV.

Key word: Diphenylamine, Tipe D-π-A, DFT, DSSC