OPTIMALISASI EFISIENSI *DYE-SENSITIZED SOLAR CELLS* (DSSCs) MELALUI MODIFIKASI ZAT WARNA MORIN: STUDI DFT (*DENSITY FUNCTIONAL THEORY*)

SKRIPSI SARJANA KIMIA

Oleh
RIFA AMELIA
BP : 1710412034

Pembimbing I : Imelda M.Si
Pembimbing II : Prof. Dr. Hermansyah Aziz

JURUSAN S1 KIMIA
FAKULTAS MATEMATIKA DAN ILMU PENGETAHUAN ALAM
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INTISARI

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Rifa Amelia (BP : 1710412034)
Imelda M.Si*, Prof. Dr. Hermansyah Aziz*
***Pembimbing**

Dye-Sensitized Solar Cells (DSSCs) merupakan sel surya generasi ketiga yang saat ini sedang dikembangkan. Pada DSSCs terdapat *sensitizer* yang berperan penting dalam proses menyerap cahaya matahari dan dikonversi menjadi energi listrik. *Sensitizer* yang digunakan biasanya berasal dari zat warna anorganik dan zat warna organik. Zat warna anorganik memiliki efisiensi yang cukup besar, tetapi terdapat banyak kelemahan, diantaranya sumber ketersediaannya yang terbatas, proses pemurniannya yang rumit, tidak ekonomis dan tidak ramah lingkungan. Oleh sebab itu dikembangkanlah zat warna organik yang bersifat ramah lingkungan, ekonomis dan sumber ketersediaannya melimpah, tetapi zat warna organik memiliki kelemahan yaitu efisiensi yang didapatkan cukup kecil. Morin merupakan salah satu zat warna organik yang pernah digunakan sebagai *sensitizer* pada DSSCs. Morin hanya bisa menyerap cahaya sampai panjang gelombang 440 nm. Pada penelitian ini morin dimodifikasi dan dianalisis menggunakan metode *Density Functional Theory* (DFT). Zat warna morin dimodifikasi menjadi tipe D-π-A, dimana morin diletakkan pada rantai akseptor dan divariasikan rantai π konyugasi dan rantai donor, kemudian dilakukan penambahan gugus pendorong dan penarik elektron. Hasil penelitian dilihat dari struktur geometri optimal, *countour Highest Occupied Molecular Orbital* (HOMO) dan *Lowest Unoccupied Molecular Orbital* (LUMO), *Molecular Electrostatic Potential* (MEP), sudut dihedral dan panjang ikatan, *bandgap* (ΔE), momen dipol, energi bebas gibbs injeksi (ΔG^{inject}) dan energi bebas gibbs regenerasi (ΔG^{reg}), panjang gelombang serapan serta nilai *Light Harvesting Efficiency* (LHE) dan tegangan (V_{oc}). Setelah dilakukan penelitian didapatkan rantai π konyugasi, rantai donor, gugus pendorong dan gugus penarik yang terbaik, dimana setelah dimodifikasi serapan cahaya panjang sampai daerah inframerah, yaitu dengan panjang gelombang sebesar 1171,94 nm dengan *bandgap* 1,36411 eV. Artinya, DSSCs yang tersensitasi zat warna baru berbasis morin ini bisa menyerap cahaya sampai malam hari dan tidak membutuhkan baterai untuk menyimpan energi.

Kata kunci : *Dye-Sensitized Solar Cells* (DSSCs), DFT, D-π-A

ABSTRACT

OPTIMIZING THE EFFICIENCY OF DYE-SENSITIZED SOLAR CELLS (DSSCs) THROUGH MODIFICATION OF MORINE COLOR: DENSITY FUNCTIONAL THEORY

by :

Rifa Amelia (BP : 1710412034)
Imelda M.Si*, Prof. Dr. Hermansyah Aziz*
***Supervisor**

Dye-Sensitized Solar Cells (DSSCs) are the third generation that are currently being developed. In the DSSC, there is a sensitizer that plays an important role in the process of absorbing sunlight and turning it into electrical energy. The sensitizers were used usually comes from inorganic dyes and organic dyes. Inorganic dyes have considerable efficiency, but there are many drawbacks, including limited resources, complicated purification process, uneconomical and not environmentally friendly. Therefore, an organic substance that is environmentally friendly, economical and has abundant sources of organic dyes has been developed, but organic dyes have a weakness, namely the management obtained is quite small. Morine is an organic dye that has been used as a sensitizer in DSSCs. Morin can only absorb light up to a wavelength of 440 nm. Branch computational chemistry is a form of chemistry that can be used as a simulator before it is synthesized in a laboratory to reduce trial and error costs. In this study using computational chemistry using the Density Functional Theory (DFT) method to increase the efficiency of the DSSC which in previous studies showed that the results using the DFT method used experimental values. In the research, morine dyes become D-π-A type dyes, which are placed on the acceptor chain and varied from the conjugate π chain and the donor chain, then the addition of the pushing and attracting groups of electrons is carried out. The results were seen from the optimal geometric structure, countour Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO), Molecular Electrostatic Potential (MEP), dihedral angles and bond lengths, bandgap (ΔE), dipole moment, free energy of gibbs injection (ΔG^{inject}) and free energy of gibbs regenaration (ΔG^{reg}), absorption wavelength and the value of Light Harvesting Efficiency (LHE) and voltage (V_{oc}). After conducting the research, it was found that the good conjugate π chain, donor chain, push and pull group, after absorption of the wavelength can absorb into the infrared region, namely 1171.94 nm with a band gap of 1.36411 eV. This means that the new morine-based dye-sensitized DSSC can be used until night time and does not require batteries to store energy.

Keywords: Dye-Sensitized Solar Cells (DSSCs), DFT, D-π-A