SYNTHESIS, CHARACTERIZATION AND ELECTRICAL CONDUCTIVITY STUDIES OF NAPHTHOYL-THIOUREA DERIVATIVES AS POTENTIAL ORGANIC LIGHT EMITTING DIODE

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Thesis Submitted in Fulfilment of the Requirement for the Degree of Master of Science in the School of Fundamental Science Universiti Malaysia Terengganu

May 2014

Abstract of thesis presented to the Senate of Universiti Malaysia Terengganu in fulfilment of the requirement for the degree of Master of Science.

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School : **School of Fundamental Science**

Thiourea motif has attracted considerably great interest in numerous applications. Molecular framework featuring thiourea derivatives as molecular wire consists of conjugated systems which promises wide range of electronic properties and suitable to be applied in molecular electronics application. Regarding to this matter, this study was carried out to determine the electrical conductivity and performance as OLED of this linear conjugated organic compounds with general formula **A**-ArC(O)NHC(S)NHAr-**D**. All synthesized compounds (**1**-**5**) were spectroscopically and analytically characterized via CHNS Elemental Microanalysis, Fourier Transform Infrared (FTIR), Ultraviolet-Visible Spectroscopy (UV-Vis), Ultraviolet-Fluorescence Spectroscopy (UV-F), ^{1}H and ^{13}C Nuclear Magnetic Resonance (NMR), Single Crystal X-Ray Crystallography Analysis, X-Ray Diffraction Spectroscopy (XRD), Thermogravimetric Analysis (TGA), Scanning Electron Microscopy (SEM) and Cyclic Voltammetry (CV) Analysis. The compounds were fabricated on ITO substrate by using electrochemical deposition method (ECD) before the electrical conductivity and performances as OLED were tested by using Four Point Probe and Two Point Probe. The Gaussian 09 Software was used to calculate the energy band gap and the electrical conductivity of the synthesized compounds to compare with experimental evaluation. The infrared spectra for **1**-**5** showed five and six significant absorptions within the expected range. From UV-Vis spectra, they show the presence of π-π^* and n-π^* electronic transitions which referred to C=O and C=S chromophores whereas from UV-F spectra, the emission spectra were observed for **1**-**5**. The ^{1}H NMR spectra exhibit all expected resonances especially for δ_H (NH). Whilst, ^{13}C NMR spectra also show expected resonances of δ_C (C=O) and δ_C (C=S) to indicate that these compounds indeed thiourea derivatives. In addition, the energy bandgaps (E_g) of all synthesized compound were measured and confirmed by theoretical calculation. The energy bandgaps (E_g) of these compounds were at around 4.49-4.72 eV and it is in a good agreement with the theoretical calculation. From the electrical conductivity study, these compounds fall in the range of semiconductor materials which is 1.61×10^{-4}-1.72×10^{-4} Scm^{-1} under dark condition. In addition, the

effect of different substituents for thiourea derivatives has been calculated due to its effective charges by using Gaussian 09 software. It is proven that the results met a good agreement with the experimental results obtained in this study. Furthermore, the performance as diode from IV curve also was carried out. The non-linear IV curves for diodes showed knee voltage in the range 0.3-1.1 V while the breakdown voltages were approximately under the reverse bias for these compounds. From these promising results, it shows that the napthoyl-thiourea derivatives can be applied as conductive and emissive layer in Organic Light Emitting Diode (OLED). Therefore, further investigation should be carried out in this type of molecular framework in many electronic devices application in the near future.

Abstrak tesis yang dikemukakan kepada Senat Universiti Malaysia Terengganu sebagai memenuhi keperluan untuk Ijazah Sarjana Sains.

SINTESIS, PENCIRIAN DAN KAJIAN KEKONDUKSIAN ELEKTRIK TERBITAN NAFTOIL-TIOUREA BERPOTENSI SEBAGAI DIOD PEMANCAR CAHAYA ORGANIK

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Pusat Pengajian : **Pusat Pengajian Sains Asas**

Motif tiourea telah menarik minat yang cukup besar di dalam pelbagai aplikasi. Kerangka molekul yang menampilkan terbitan thiourea sebagai wayar molekul yang terdiri daripada sistem terkonjugat yang menjanjikan pelbagai ciri-ciri elektronik yang sesuai digunakan dalam aplikasi elektronik molekul. Merujuk kepada perkara ini, kajian ini telah dijalankan untuk menentukan kekonduksian elektrik dan prestasi sebagai OLED daripada sebatian organik terkonjugasi lurus dengan formula am **A**-ArC(O)NHC(S)NHAr-**D**. Semua sebatian yang disintesis (**1**-**5**) telah dicirikan secara spektroskopi dan analitikal melalui Analisis Unsur Mikro CHNS, Sinar Inframerah Penukaran Fourier (FTIR), Spektroskopi Ultra-Lembayung Sinar Tampak (UV-Vis), Spektroskopi Ultra-lembayung Pendaflour (UV-F), ^{1}H dan ^{13}C Resonans Magnetik Nukleus (NMR), Analisis Kristalografi Hablur Tunggal, Spektroskopi Pembelauan Sinar X (XRD), Analisis Gravimetri Terma (TGA), Mikroskop Pengimbas Elektron (SEM) dan Analisis Voltametri Kitaran (CV). Sebatian yang telah difabrikasikan ke atas substrat ITO dengan menggunakan kaedah pengelektronapan (ECD) sebelum kekonduksian elektrik dan prestasi sebagai OLED diuji dengan menggunakan Penduga Empat Titik dan Penduga Dua Titik. Perisian Gaussian 09 telah digunakan untuk mengira jurang jalur tenaga dan kekonduksian elektrik sebatian yang disintesis untuk membuat perbandingan dengan penilaian eksperimen. Spektra inframerah untuk sebatian **1**-**5** menunjukkan lima dan enam serapan penting dalam julat yang dijangkakan. Daripada spektra UV-Vis, kehadiran peralihan elektronik π-π^* and n-π^* ditunjukkan kepada kromofor C=O dan C=S manakala spektra UV-F, spektra pancaran telah diperhatikan bagi sebatian **1**-**5**. Spektra ^{1}H NMR telah mempamerkan semua resonan yang dijangka terutamanya bagi δ_H (NH). Sementara itu, ^{13}C NMR juga menunjukkan resonan yang dijangkaan iaitu δ_C (C=O) dan δ_C (C=S) yang menunjukkan bahawa sebatian ini sememangnya terbitan tiourea. Di samping itu, jurang jalur tenaga (E_g) daripada semua sebatian yang disintesis telah dinilai dan disahkan dengan pengiraan teori. Jurang jalur tenaga sebatian ini adalah sekitar 4.49-4.72 eV dan sangat bertepatan dengan pengiraan teori. Dari kajian kekonduksian elektrik, sebatian-sebatian

ini adalah tergolong di dalam julat bahan semikonduktor iaitu $1.61x10^{-4}$-$1.72x10^{-4}$ Scm^{-1} dalam keaadaan gelap. Di samping itu, kesan gantian berlainan yang berbeza bagi terbitan tiourea telah dinilai berdasarkan cas efektif dengan menggunakan perisian Gaussian 09. Ini membuktikan bahawa keputusan teori sangat bertepatan dengan keputusan eksperimen yang diperolehi dalam kajian ini.Tambahan pula, prestasi OLED dari lengkungan IV juga telah dijalankan. Lengkungan IV bukan lurus untuk OLED menunjukkan voltan "knee" dalam julat 0.3-1.1 V manakala voltan "breakdown" adalah didalam pincang sonsang untuk sebatian-sebatian ini. Daripada keputusan yang memberangsangkan, ini menunjukkan bahawa terbitan naftoil-tiourea boleh digunakan sebagai lapisan konduktif dan pemancar dalam Diod Pemancar Cahaya Organik (OLED). Oleh itu, kajian lanjutan perlulah dijalankan pada jenis kerangka molekul ini dalam pelbagai penggunaan peralatan elektronik di masa hadapan.