UNIVERSITI TEKNOLOGI MARA

COMPUTATIONAL AND CHARACTERIZATION STUDIES OF NON-CONJUGATED POLY(N-VINYLCARBAZOLE) BLENDS AS HOST POLYMER FOR PHOSPHORESCENCE EMISSION

AHMAD NAZIB BIN ALIAS

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AUTHOR'S DECLARATION

I declare that the work in this thesis was carried out in accordance with the regulations of Universiti Teknologi MARA. It is original and is the results of my own work, unless otherwise indicated or acknowledged as referenced work. This topic has not been submitted to any other academic institution or non-academic institution for any degree or qualification.

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Name of Student	:	Ahmad Nazib Alias
Student I.D. No.	:	2010656824
Programme	:	Doctor of Philosophy in Science
Faculty	:	Applied Science
Thesis Tittle	:	Computational and Characterization Studies of Non-Conjugated Poly(N-vinylCarbazole) Blends As Host Polymer For Phosphorescence Emission
Signature of Candidate	:	.....
Date	:	March 2015

ABSTRACT

Polarized absorption, optical dielectric spectra, absorption excitation and emissions spectra of blended poly (N-carbazole) (PVK) with poly(vinylidene fluoride-co-hexafluoropropene) (PVDF-HFP) and polyvinylpyrrolidone (PVP) in the same composition have been investigated. The electronic structure has been calculated using extrapolation of oligomer method by semiempirical Zerner Modified Intermediate Neglect of Differential Overlap (ZINDO) calculation. Polymer coating was carried out using doctor blade technique on a quartz substrate. Polarized absorption, optical dielectric spectra, absorption excitation and emission spectra reveal that there are significant different results obtained between PVK, PVK:PVP and PVK:PVDF-HFP. The electronic parameters such as absorption edge (E_e), allowed direct bandgap (E_d), allowed indirect bandgap (E_i) and Urbach edge (E_u) were calculated using Tauc/Davis-Mott Model. The dispersion behavior of polymer blending has been discussed using the Wemple–DiDomenico and Sellmeier model. The luminescence excitation and emission spectra have also been evaluated and results reveal that significant changes occur in the spectrum with different polymer blends. PVK:PVP has the highest emission intensity and low Stokes shift followed by PVK:PVDF-HfP and PVK. The existing state of gap was calculated using AC conductivity. This result has further been used to predict the factor that affected the recombination mechanism. The luminescence mechanism due to energy transfer has been supported using electronic calculation and Fourier transforms infrared spectroscopy. Resonance transfer of electronic excitation energy from sensitizer (donor) to activator (acceptor) has been modeled by using coupling resonance approach. The highest intensity of polymer blend (PVK:PVP) has futher been investigated by changing the composition ratio. The polymer blending systems consist of blended PVK with PVP (PVK:PVP) in different weight ratios namely S1 (9:1), S2 (8:2), S3 (7:3), S4 (6:4), S5 (5:5), and S6 (4:6). S5 show the maximum excitation and emission properties. The maximum of excitation and emission energy are discrepant non-linearly with the composition ratio. The emission spectra of Europium complex blended with PVK, PVK:PVDF-HfP and PVK:PVP has also been investigated. The emission spectra for all samples show the character of Eu complex. Eu complex blended with PVK shows the highest transition, followed by PVK:PVDF-HfP and PVK:PVP. This shows that the type of host polymer strongly depends upon the type of host polymer blended in Eu complex. Based on singlet-triplet energy levels and phosphorescence yield calculation, there are significant changes in the phosphorescence emission intensity when different host polymers are used.

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