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Electroluminescent Properties of Pentacene Derivatives having a Naphthalene Moiety

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We synthesized 6,13-Di-phenyl-pentacene (DPP), 6,13-Di-naphthalen-1-yl-pentacene (1-DNP) and 6,13-Di-naphthalen-2-yl-pentacene (2-DNP). Photoluminescent properties, electroluminescent properties and molecular interaction between 1-DNP and 2-DNP were discussed. EL spectra of synthetic materials showed similar tendency of EL maximum value at around 621/628 nm and 669/675 nm. EL efficiency of Alq $_3$ doped with 2-DNP also showed better efficiency of 0.67 cd/A and 0.13l m/W compared to DPP and 1-DNP's due to different molecular interaction.

Keywords: light-emitting diode; pentacene

INTRODUCTION

For the past decades, great successes have been made in the field of organic light-emitting diodes (OLEDs). Green and blue OLEDs with high efficiency, good color coordinate value, and long lifetime have been reported [1,2]. Numerous red fluorescent materials for OLEDs have been reported, but it is still not satisfactory [3–5]. Presently, most high-performance red OLEDs are made by doping a red dye into a suitable host [6,7]. The reported dopants include pyran-containing

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compound [5,8,9], porphyrin compound [4,10–12], europium complexes [13–15] and diphenylpentacene compound [16–18].

In order to increase red OLED performance, we need to consider the spacial arrangement of chromophore molecule like 9,10-di-(2-naphthyl) anthracene (ADN) and 2-methyl-9,10-di-(2-naphthyl)anthracene (MADN) [19,20]. Therefore, in this paper, we compare the EL properties of pentacene derivatives with the different spacial arrangement by through naphthalene moiety.

We reported the synthesis and photoluminescent (PL) properties of new 6,13-Di-naphthalen-1-yl-pentacene (1-DNP) and 6,13-Di-naphthalen-2-yl-pentacene (2-DNP) as pentacene derivatives [18]. In here, we report electroluminescent (EL) properties of 6,13-Di-phenyl-pentacene (DPP), 1-DNP and 2-DNP.

EXPERIMENTAL

Synthesis

Synthesis of 1-DNP and 2-DNP synthetic procedure of 1-DNP and 2-DNP was reported in previous paper [18] (see Scheme 1).

(4) 1 H NMR (δ ,ppm): 8.35(s, 4H), 7.80(m, 8H), 7.73(m,2H), 7.69 (m, 4H), 7.30(q, 4H) FAB-mass: 430.

SCHEME 1 Synthetic route of pentacene derivatives (DPP(4), 1-DNP(5), 2-DNP(6)).

- (5) 1 H NMR (δ ,ppm): 8.21(t, 2H), 8.10(m, 4H), 7.99(d, 1H), 7.86(d, 2H), 7.78(d, 3H), 7.58(d, 2H), 7.53(t, 3H), 7.23(d, 4H), 7.15(m, 5H), FAB-mass: 530.
- (6) 1 H NMR (δ ,ppm): 8.21(t, 2H), 8.10(m, 4H), 7.99(d, 1H), 7.86(d, 2H), 7.78(d, 3H), 7.58(d, 2H), 7.53(t, 3H), 7.23(d, 4H), 7.15(m, 5H), FAB-mass: 530.

Fabrication of OLED

The devices were fabricated on glass substrates. The organic layer were vacuum-deposited using thermal evaporation at a vacuum base pressure of 5.0×10^{-6} Torr, the rate of deposition being 1Å per second to give an emitting area of $9\,\mathrm{mm}^2$ and aluminum layer was continuously deposited with same vacuum condition. The multilayer structure consists the following layers: Al as an anode(200 nm), 2-TNATA as a hole injection(60 nm), NPB as a hole transport layer(15 nm), emitting layer(EML), electron transport layer(ETL), LiF as an electron injection layer(1 nm), Al as a cathode(20 nm).

Measurements

Perkin Elmer luminescence spectrometer LS55 (Xenon flash tube) was used for electroluminescence spectroscopy. Current-voltage(I-V) characteristics of the film in plane were measured using Keithley 2410 electrometer. Light intensity was obtained by Minolta CS-100.

RESULTS AND DISCUSSION

In previous paper, we reported red PL tendency under the different solute concentration and that 2-DNP has relatively lower packing ratio and molecular interaction than 1-DNP's because of steric hinderance of 2-naphthyl bulky group. These molecular interaction differences between 1-DNP and 2-DNP confirm with melting point result. There is no EL light emission in OLED devices which were fabricated with synthetic materials of DPP, 1-DNP and 2-DNP as host emitting material. In this study, PL and EL properties of DPP, 1-DNP and 2-DNP as doping agent and molecular interaction between 1- and 2-position were investigated.

According to UV spectrum of these pentacene derivatives in our previous paper, the maximum wavelength values were about 482, 517, 554 and 600 nm, which overlapped well with PL spectrum of Alq₃. Therefore we have applied synthesized pentacene derivatives as dopant to Alq₃ host material.

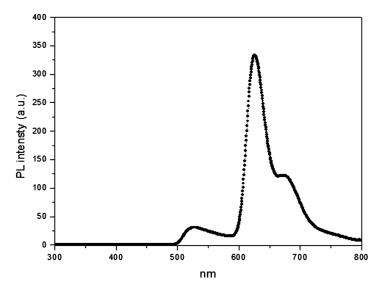


FIGURE 1 Photoluminescence spectra of Alq₃ film doped with 2-DNP.

Figure 1 shows PL spectrum of Alq₃ film doped with 2-DNP. DPP and 1-DNP also showed very similar PL shape with 2-DNP. It showed PL maximum values of 623 and 674 nm and Alq₃ residual peak at 529 nm which is not fully transferred from host to dopant.

Figure 2 shows EL spectra of ITO/2-TNATA(50 nm)/NPB(20 nm)/ Alq_3 doped with 1-DNP or 2-DNP(30 nm)/ Alq_3 (30 nm)/LiF/Al. These devices showed similar tendency of EL maximum value at around 621/628 nm and 669/675 nm. There was Alq_3 residual EL peak at around 529 nm and DPP also showed almost same EL spectrum as 1-DNP and 2-DNP. We also find out I-V characteristics of these kinds of devices. 2-DNP device achieved better I-V characteristics than 1-DNP's as shown in Figure 3.

In PL results, we observed the difference of molecular interaction as pending site of naphthalene moiety. In EL spectra, there is similar EL shape as 1-position or 2-position of naphthalene, but EL efficiency data shows different result in EL devices. Luminescence efficiency and power efficiency summarized in Table 1.

Standard green efficiency of ITO/2-TNATA(60 nm)/NPB(15 nm)/ $Alq_3(70 \text{ nm})/LiF(1 \text{ nm})/Al$ (200 nm) device shows 4.42 cd/A and 2.39 lm/W at 10 mA/cm^2 with (0.309, 0.514) CIE color coordinate value in our device system. The values of standard green EL device efficiency and these device efficiency were relatively lower than other group's but these values were reliable because of good reproducibility and equal

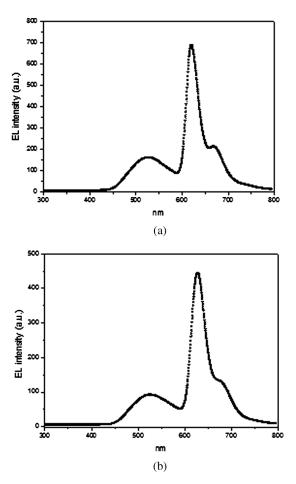


FIGURE 2 Electroluminescence spectra of 1-DNP(a), 2-DNP(b) device; ITO/2-TNATA(50 nm)/NPB(20 nm)/Alq $_3$ doped with 1-DNP or 2-DNP(30 nm)/Alq $_3$ (30 nm)/LiF/Al.

comprision under same experiment condition. EL efficiency of 2-DNP also showed better efficiency of 0.67 cd/A and 0.13 lm/W compared to DPP and 1-DNP's. The EL efficiency of pentacene with naphthalene moiety was affected by molecular interaction of steric effect. We believe that molecular interaction maybe an important factor for increasing EL efficiency in host-dopant EL emitting system because there is an obvious energy transfer process from host to dopant materials. EL efficiency of 2-DNP is 4 times higher than DPP's of Kafafi *et al.* [16], which is due to spacial arrangement. In 9,10-di-(2-naphthyl)anthracene (ADN) and

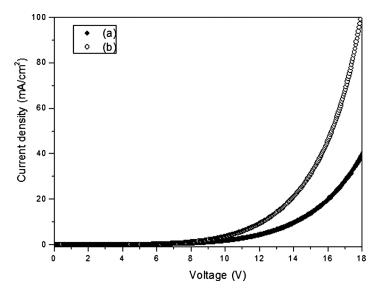


FIGURE 3 I-V curve of 1-DNP (solid, a), 2-DNP (open, b) device; ITO/2-TNATA(50 nm)/NPB(20 nm)/Alq $_3$ doped with 1-DNP or 2-DNP(30 nm)/Alq $_3$ (30 nm)/LiF/Al.

2-methyl-9,10-di-(2-naphthyl) anthracene (MADN) case of Chen *et al.*, the symmetry and close molecular packing of ADN is disrupted by methyl substituent in the space group which results in the increase of the intermolecular distance [19,20]. It caused higher EL efficiency and longer life-time in device performance.

Additionally we analyzed electrochemical stability of synthesized compounds as cyclic voltammetry(CV), because electrochemical stability is one of the key issues, in order to improve life time of device.

CV properties of these derivatives in solid film states will be reported in the other paper.

TABLE 1 Efficiency and Color Coordinates of Pentacene Derivatives

Dopant	Luminescence efficiency (cd/A)	Power efficiency (lm/W)	Color cooridinate
DPP	0.16	0.052	x = 0.58
1-DNP	0.027	0.0047	y = 0.37 x = 0.56
2-DNP	0.67	0.13	y = 0.38 $x = 0.56$
			y = 0.38

CONCLUSIONS

EL spectra of ITO/2-TNATA($50\,\mathrm{nm}$)/NPB($20\,\mathrm{nm}$)/Alq₃ doped with 1-DNP or 2-DNP($30\,\mathrm{nm}$)/Alq₃($30\,\mathrm{nm}$)/LiF/Al showed similar tendency of EL maximum value at around $621/628\,\mathrm{nm}$ and $669/675\,\mathrm{nm}$. EL efficiency of 2-DNP also showed better efficiency of $0.67\,\mathrm{cd/A}$ and $0.13\,\mathrm{lm/W}$ compared to DPP and 1-DNP's. The EL efficiency of pentacene with naphthalene moiety was affected by molecular interaction of steric effect. We believe that molecular interaction could be an important factor for increasing EL efficiency in host-dopant EL emitting system because there is an obvious energy transfer process from host to dopant materials. EL efficiency of 2-DNP is 4 times higher than DPP's, which is due to spacial arrangement. We verified the important factor of spacial arrangement of chromophore with substituent moiety in EL performance.

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