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Asymmetric 1,3,4-oxadiazole derivatives containing naphthalene and stilbene units: Synthesis, optical and electrochemical properties

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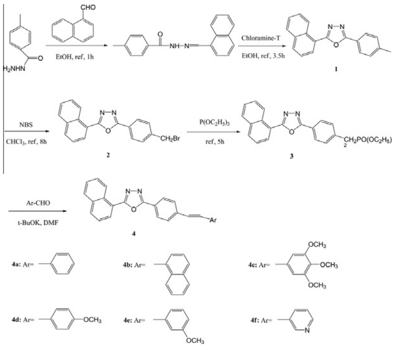
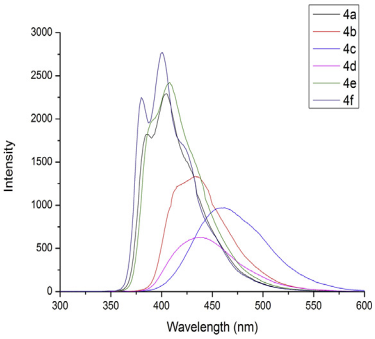
HIGHLIGHTS

- Asymmetrical 1,3,4-oxadiazole dyes were efficiently synthesized.
- Structure–optical properties relationships were investigated.
- The compounds exhibit bright violet–blue emission with high fluorescence quantum yields.
- The high HOMO levels (−5.17 to −5.03 eV) are beneficial for hole-transporting.

GRAPHICAL ABSTRACT





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ABSTRACT

Six novel asymmetric 1,3,4-oxadiazole derivatives containing naphthalene and stilbene units have been efficiently synthesized and characterized by FT-IR, ^{1}H NMR, ^{13}C NMR, mass spectrometry and elemental analysis. The UV–vis absorption maximum wavelength, fluorescence excitation wavelength, fluorescence emission wavelength and fluorescence quantum yield were measured in dilute tetrahydrofuran solution. The solvent effect was also studied. The HOMO and LUMO levels of these compounds were calculated by density functional theory (DFT) (B3LYP, 6-31G*) method and cyclic voltammetry. They emit bright violet to blue emission with high fluorescence quantum yields (0.23–0.94) and large Stokes shifts (53–102 nm). These compounds possess high HOMO levels (−5.03 to −5.17 eV) and suitable band gaps, indicating that they could be benefit for hole injection. The results show that they have a potential for application in optoelectronic materials.

Introduction

Organic dyes have been extensively investigated for versatile applications in coloring textiles, dye laser device, organic light emitting diodes and electroluminescent displays [1–4]. 1,3,4-Oxadiazoles are well known not only for their attraction in medicinal and pesticide chemistry [5–9], but also for their outstanding photoelectric properties such as electron-transporting capabilities, durability stability and high fluorescence quantum yields [10–12]. Many symmetrical 1,3,4-oxadiazole derivatives have actually been synthesized to use as TPA materials, polymers and organic electroluminescent (EL) devices [13–15]. However, it is well known that the large π-symmetrical system leads to poor solubility, which limits their synthesis, characterizations and applications [16]. Therefore, the synthesis of asymmetric 1,3,4-oxadiazole derivatives with high efficiency emitting are still in demand.

Naphthalene chromophore is an attractive π center, not only because it is planar, but it is also an excellent fluorophore. Though a great deal of excellent work has been reported on the naphthalene derivatives as organic electroluminescent (EL) materials [17,18], it is still meaningful to extend the research of such

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materials. The naphthyl π systems attached to electron withdrawing groups are found to be effective photosensitive, and exhibit good electrochemical and optical properties [19,20].

The π-conjugated organic materials have attracted much attention owing to the increasing development of potentially active components for a wide range of electronic and optoelectronic devices [21]. Stilbene fluorescent compounds are an important class of fluorescent compounds with strong UV absorption, distinctive fluorescence emission and large Stokes shifts [22–24], which have developed as optical brighteners, TPA materials and electroluminescent materials [25–27]. The introduction of stilbene unit into the oxadiazole dyes not only builds a π-conjugated bridge, but also leads to a larger molecular length, which would make the electron-pair in the highest occupied molecular orbit possess a higher energy; the electron-pair could be excited easily to transit into a higher orbit [28].

On the basis of our previous studies on organic fluorescent materials [15,29,30], herein, we report six novel violet–blue asymmetric 1,3,4-oxadiazole dyes containing naphthalene chromophore with stilbene unit. As expected, the new dyes have good photoelectric properties such as strong fluorescence intensity, high HOMO levels and suitable band gaps. In addition, these compounds possess high fluorescence quantum yields, large Stokes shift and good electrochemical properties. The results will increase the knowledge to design and synthesis novel asymmetric 1,3,4-oxadiazole derivatives based on stilbene with excellent photophysical properties.

Experimental

Materials and instruments

All starting materials and reagents were commercially available and used without further purification. All solvents were carefully dried and freshly distilled according to common laboratory techniques. Melting points were determined using RY-1 melting point apparatus and were uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 on a Bruker AVANCE-400 MHz NMR spectrometer using TMS as internal standard. FT-IR spectra were measured as KBr pellets on a Bruker TENSOR 27 in the region of 4000–400 cm^{-1}. Mass spectra were obtained with a Bruker Esquire HCTplus (APCI). Elemental analyzes were performed on a Vario EL cube V2.1.0 elemental analyzer. UV–vis absorption spectra were recorded on a Hitachi UV-3010 spectrophotometer. Fluorescence spectra were obtained on a Hitachi F-4500 spectrophotometer at room temperature. The purity of the compounds was confirmed by TLC on silica gel 'G'-coated glass plates. Cyclic voltammetry was carried on a CHI830B electrochemical analyzer with three-electrode cell (Pt working electrode, Pt wire counter electrode and Ag/AgCl reference electrode) in CH_2Cl_2 solution in the presence of tetrabutylammonium hexafluorophosphate (0.1 M) as supporting electrolyte.

Measurements

The fluorescence quantum yields (Φ) were determined according to the literature method [31,32].

$$\Phi_x = (A_s \times F_x \times n_x^2 \times \Phi_s)/(A_x \times F_s \times n_s^2)$$

Here, A is the absorbance at the excitation wavelength, F is the area under the fluorescence curve, n is the refraction index. Subscripts s and x refer to the standard and to the sample of unknown quantum yield, respectively. Quinine sulfate in 0.5 M sulfuric acid was used as fluorescence standard (Φ = 0.546) [33].

Synthesis

The designed synthetic route for the target compounds are depicted in Scheme 1. The synthesis procedure and the analytical data of the compounds can be seen in Supplementary material.

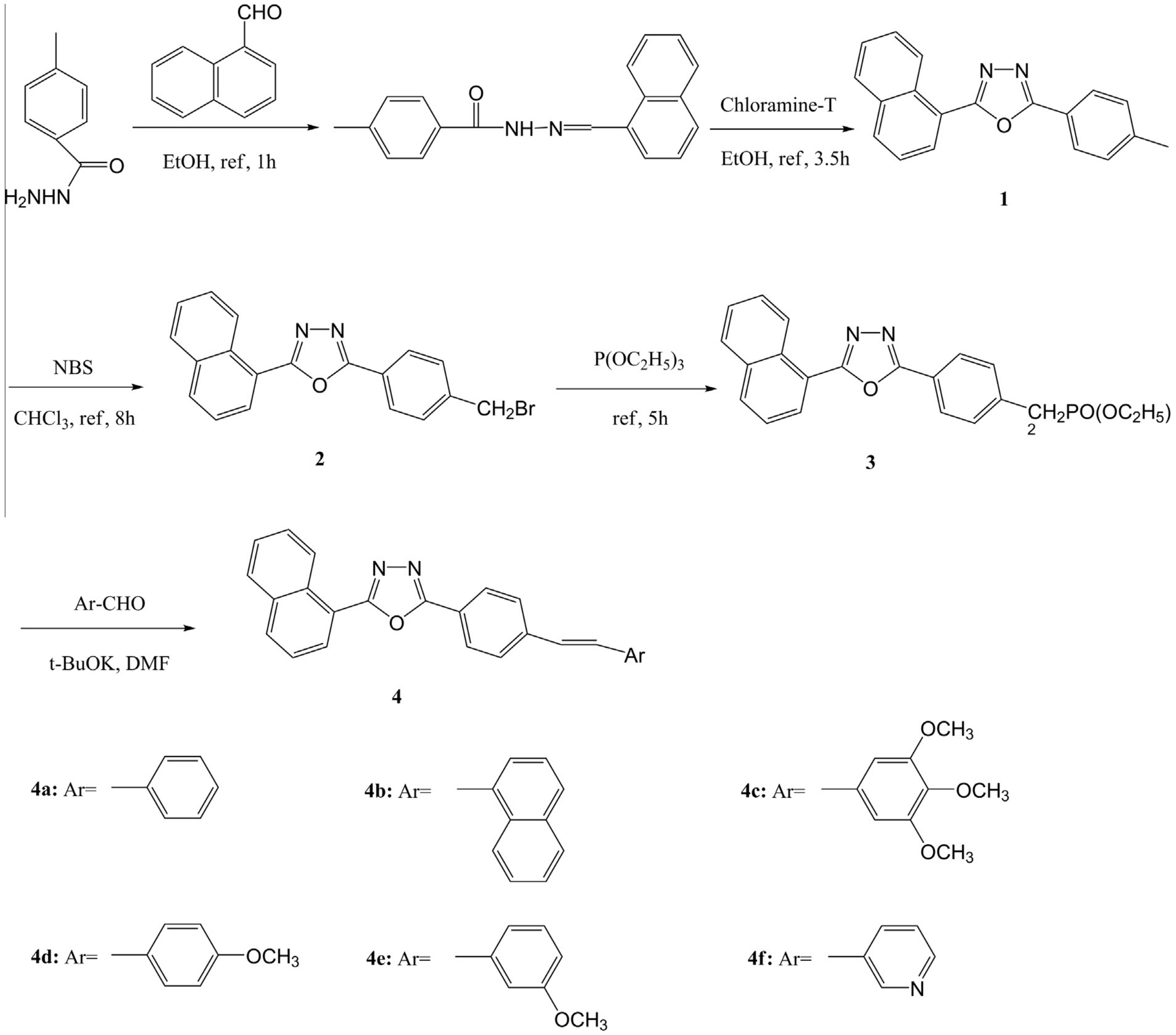
Results and discussion

The synthesis and characterization

The reaction steps for the synthesis and the structures of the target molecules are shown in Scheme 1. Intermediate **1** was prepared through the oxidative cyclization of hydrazones derived from aromatic aldehydes and 4-methylbenzohydrazide by chloramine-T, and then reacted with N-bromosuccinimide under the catalysis of benzoyl peroxide to get compound **2**. Compound **2** and triethyl phosphite were mixed to prepare compound **3** through esterification. We then used compound **3** to react with various aldehydes, via Wittig–Horner reaction, to get a series of asymmetric 1,3,4-oxadiazole derivatives. Wittig–Horner reaction is an important synthetic route for the formation of an olefin functional group. The reaction procedure is convenient, takes place under mild conditions, and gives good yields. All new compounds were confirmed by ^{1}H NMR, ^{13}C NMR, MS, FT-IR and elemental analysis. The spectroscopic data of products are in accordance with the assigned structures. The FT-IR spectra show weak bands or shoulders located at 3100–3000 cm^{-1}, a strong band at 1606–1608 cm^{-1} and at 1530 cm^{-1} which is assigned to aromatic C—H, C=N and aromatic C—C, respectively. IR spectra of **4c–4f** exhibit the stretching band at 2963–2826 cm^{-1} assigned to aliphatic groups and at 1130 cm^{-1} corresponding to aromatic C—O—C groups. Furthermore, the appearance of moderate intensity sharp C=C vibration band at 963 cm^{-1} indicate the existence of stilbene, which suggests the molecules are trans-structure [34]. In the ^{13}C NMR spectra, because of the electron withdrawing ability of the imine group, two resonance peaks appear at around 165 and 163 ppm which are assigned to two C atoms of 1,3,4-oxadiazole. In the ^{1}H NMR spectra of target compounds, the total number of hydrogen atoms is in good agreement with the proposed structure. The protons of the naphthyl and phenyl attached to oxadiazole are shifted to higher chemical shifts (δ = 9.30 and 8.20 ppm) due to the electron-withdrawing ability of the oxadiazole lead to a decrease of the electron density. The doublet of CH=CH with 16.0–16.7 Hz coupling constant in the ^{1}H NMR spectra of target compounds indicate the vinyl is trans-structure, but the multiplet of CH=CH appears in **4b** and **4e** owing to the doublet of vinyl is overlapped with the peaks of aromatic-H. In the mass spectra, the presence of characteristic molecular ion peaks [M + 1] confirm the proposed structures.

Optical properties

The optical data of the compounds were summarized in Table 1. The UV–vis absorption spectra and emission spectra of the compounds are given in Figs. 1 and 2 (1×10^{-5} mol L^{-1} in tetrahydrofuran solution). It can be observed that these compounds have similar absorption spectra owing to their molecular structures. As is apparent in Fig. 1, all derivatives exhibit intense CT absorptions in the visible region from 345 nm to 357 nm, which is attributed to an intramolecular charge transfer transition ($S_0 \rightarrow$ CT). The compound **4c** exhibits the largest maximum absorption peak at 357 indicating the introduction of electron-donating methoxy group into the phenyl results in bathochromic shift. It is also noted that the red-shift effect of the methoxy substituent is related to the numbers of methoxy and the substituent position. When the



Scheme 1. The synthetic route of new target compounds.

Table 1
UV–vis and fluorescent parameters of target compounds.

Compound	λ_{max} (nm)[a]	$10^{-4}\varepsilon_{max}$ (L mol^{-1} cm^{-1})[a]	λ_{ex} (nm)[a]	λ_{em} (nm)			Stockes shifts (nm)[b]	Φ_x[c]
				DMSO	THF	$CHCl_3$		
4a	345	4.61	348	417	404	406	56	0.82
4b	352	4.24	358	450	434	430	76	0.59
4c	357	4.87	360	500	462	450	102	0.56
4d	356	4.88	362	467	437	430	75	0.23
4e	349	5.10	351	423	408	408	57	0.84
4f	346	5.17	348	407	401	402	53	0.94

[a] Solution in 10^{-5} mol L^{-1} THF.
[b] Stokes shifts = $\lambda_{em} - \lambda_{ex}$.
[c] The fluorescence quantum yields were measured in THF using Quinine sulfate in 0.5 M sulfuric acid as the standard.

phenyl ring is substituted with an $-OCH_3$ group at *m*- and *p*-position, the λ_{max} values are shifted to 349(**4e**) and 356(**4d**) nm, respectively. This can be explained by the decreasing electron donating effect of the $-OCH_3$ group attached to the *m*-position. Compared with **4a**, compound **4b** exhibits a red shifted absorption maximized at 352 nm due to longer conjugation length and larger delocalized system. Compound **4a** and **4f** have the similar maximum absorption peaks, indicating that pyridine ring has a limited effect on their electronic energy levels.

As can be seen in Table 1 and Fig. 2, all of the compounds exhibit strong violet to blue emission with the maximum peaks varying from 401 to 462 nm in THF solution. The blue light-emitting materials play a particularly significant role in the development of OLEDs, because they can not only be used as a blue light source, but also be utilized to generate light of green and red color by energy cascade to a suitable emissive dopant [35,36]. Moreover, their emission range can be tuned by changing the nature of the peripheral substituting groups. It is well known that a strong electron donor could help to stabilize charge-transfer excited state and cause red shift. The compound **4b** exhibits bright blue emission with peak at 434 nm, which is bathochromically shifted with respect to that of **4a** because of the larger conjugation of naphthyl. The fluorescence emission peaks for **4c**, **4d** and **4e** are gradually red shifted due to the increased electron density by -OCH_3. The Stokes shifts for all the compounds are large, ranging from 53 to 102 nm. The large Stokes shift means a small overlap between the absorption and fluorescent spectra, which is an advantage in luminous material [37]. These compounds exhibit different emission behaviors by changing the nature of the polarity of the solvents. With increasing polarity of the solvent, their fluorescence spectra show bathochromic shifts. For example (Fig. 3), λ_{max} of **4c** is located at 450 nm in $CHCl_3$ and red-shifted to 500 nm in DMSO, indicating that it is more polarity in the excited state than in the ground state. These demonstrate that the polarity of the solvent plays an important role on the photophysical properties in such strong donor–acceptor systems. The fluorescence quantum yields of the compounds are in the range of 0.23–0.94. Concerning **4a** and **4b**, the $\boldsymbol{\Phi}_x$ values decrease with the increase of conjugation ascribed to torsion occur around the olefin bond because of the steric hindrance. It can be found that **4c** and **4d** were lower than **4a**, which might be attributed to the introduction of methoxy affecting the planarity of the molecules.

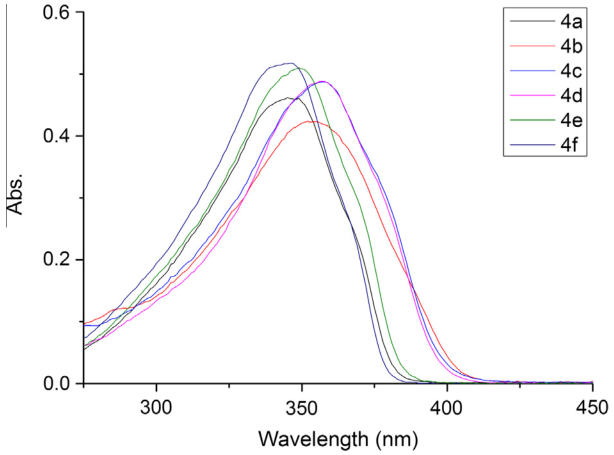


Fig. 1. The absorption spectra of target compounds (1×10^{-5} mol L^{-1} in THF).

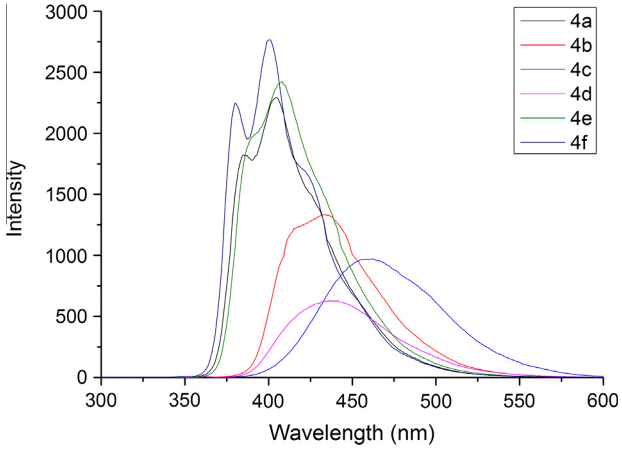


Fig. 2. The emission spectra of target compounds (1×10^{-5} mol L^{-1} in THF).

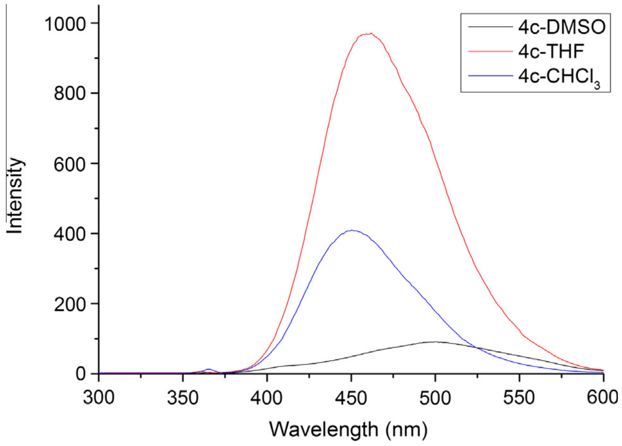


Fig. 3. The emission spectra of compound **4c** in different solvents (1×10^{-5} mol L^{-1}) as sample.

Theoretical calculations

The ground-state geometries and electronic structures of the target compounds were calculated with Gaussian 09 software, using density functional theory (DFT) at the (B3LYP)/6-31G* level

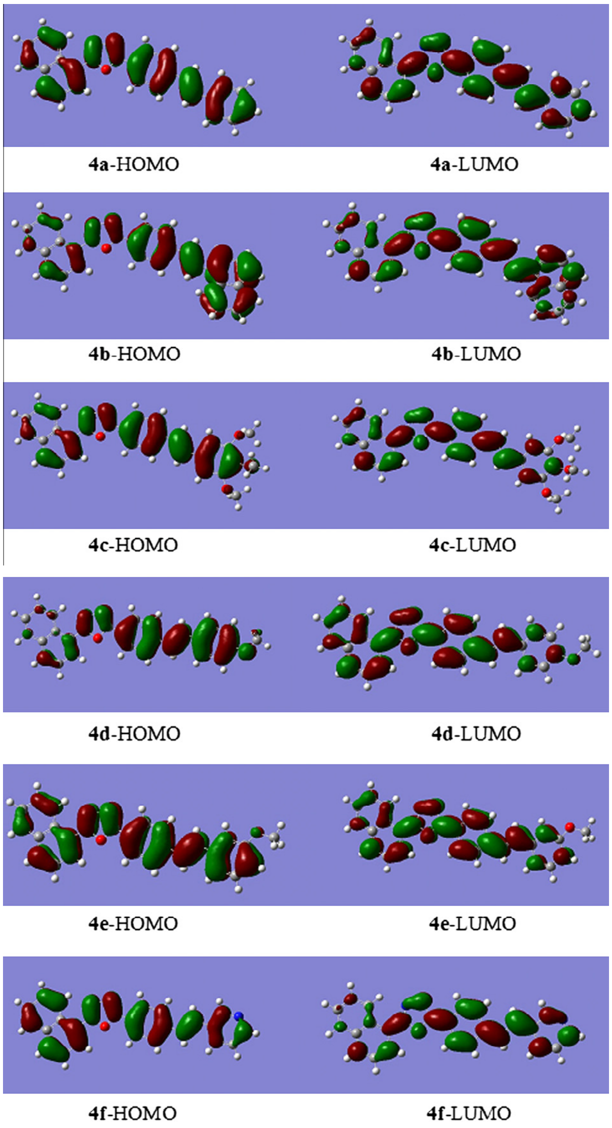


Fig. 4. Optimized geometric structure and frontier molecular orbital profiles of compounds.

Table 2
Electrochemical properties of target compounds.

Compound	HOMO (eV)[a]	LUMO (eV)[a]	Band gap (eV)[a]	E_{ox} (eV)[b]	HOMO (eV)[c]	LUMO (eV)[c]	E_g (eV)[d]
4a	−5.55	−2.04	3.51	0.74	−5.14	−1.99	3.15
4b	−5.48	−2.06	3.42	0.70	−5.10	−2.18	2.92
4c	−5.48	−2.02	3.46	0.63	−5.03	−2.12	2.91
4d	−5.31	−1.93	3.48	0.69	−5.09	−2.07	3.02
4e	−5.51	−2.00	3.51	0.69	−5.09	−1.90	3.19
4f	−5.70	−2.19	3.51	0.77	−5.17	−1.97	3.20

[a] DFT/B3LYP calculated values.
[b] Oxidation potential in CH_2Cl_2 (10^{-3} mol L^{-1}) containing 0.1 mol L^{-1} $(n\text{-}C_4H_9)_4NPF_6$ with a scan rate of 0.05 V s^{-1}.
[c] $E_{HOMO} = -(E_{ox} + 4.4)$ eV, and $|E_{LUMO}| = |E_{HOMO}| - E_g$.
[d] Energy gap was estimated from the absorption edge.

[38]. The electron-density distribution of the highest occupied molecular orbit (HOMO) and the lowest unoccupied molecular orbit (LUMO) of ground-state optimized structures are shown in Fig. 4. The calculated energy levels are listed in Table 2. Fig. 4 shows that all compounds have good coplanar configurations except for **4b**, which implies that these compounds have a large π-delocalization. And the dihedral angle in **4b** between naphthyl and vinyl is 149.3°. Generally, the more coplanar or rigid structure the higher fluorescence efficiency is. It can be observed that the HOMOs are spread over the entire conjugated molecules ascribe to π orbital, while the LUMOs are mainly localized on the oxadiazole ring, two adjacent phenyl rings and stilbene ascribe to π^* orbital, suggesting that the naphthyl and the donor-substituted groups contribute to enhance the charge mobility of the target compounds. This illustrates that these molecules possess strong intramolecular charge transfer ability between donor unit and acceptor moiety. Concerned on **4d**, we can observe that the introduction of methoxy group changes the electron density distribution of HOMO. The calculated HOMO and LUMO energy levels of the compounds are from −5.70 to −5.31 eV and from −2.19 to −1.93 eV, respectively. The HOMO energy levels of the target compounds are close to the most well-known hole-transporting materials such as TPD (−5.73 eV) and NBP (−5.30 eV), indicating that they might be beneficial for the hole-transporting [17,39]. Compared with the commonly used cathode barium (−2.2 eV), the low LUMO energy of these compounds (−2.19 to −1.93 eV) have a small barrier to accept electrons from the cathode [40]. The theoretical band gaps are in range of 3.42–3.51 eV closed to the most famously blue-emitting diode ZnO NWs (3.37 eV), which indicate that the target compounds may be used as a host material for blue emitters [41–43].

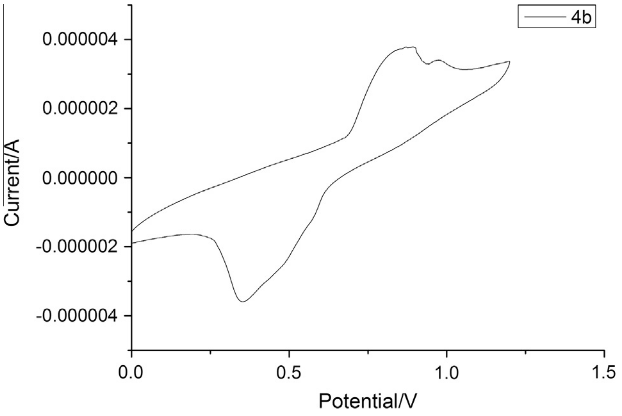


Fig. 5. Cyclic voltammogram of compound **4b** as sample, in 0.1 mol L^{-1} Bu_4NPF_6–$CHCl_3$, scan rate 50 mV s^{-1}.

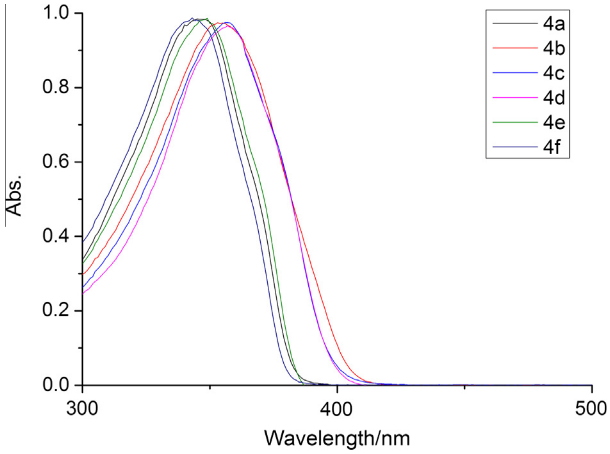


Fig. 6. UV–vis absorption spectra of **4a**, **4b**, **4c**, **4d**, **4e** and **4f** in CH_2Cl_2 solution.

Electrochemical properties

The electrochemical properties of compounds **4a–4f** were investigated by cyclic voltammetry in CH_2Cl_2 with 0.1 M tetrabutylammonium hexafluorophosphate as supporting electrolyte at scan rate of 50 mV s^{-1} under nitrogen atmosphere. Fig. 5 shows that compounds exhibit reversible oxidation process with onset oxidation potential of 0.63–0.77 V. The HOMO and LUMO energy levels were deduced from the following equations: $\mathrm{HOMO} = -(E^{ox}_{onset} + 4.4)$, $E_g = 1240/\lambda_{onset}$ (see Fig. 6) and $|\mathrm{LUMO}| = |\mathrm{HOMO}| - E_g$. As shown in Table 2, HOMO levels of compounds are range from −5.03 to −5.17 eV, which are higher than the most widely used HTM NPB (−5.40 eV) [44]. The higher HOMO energy the smaller energy barrier between the interface of ITO and the target compounds, and resulted in higher hole injection efficiency and lower joule heat [45]. These compounds possess small bang gaps (2.91–3.20 eV), which are smaller or close to the blue emitter DPB (3.20 eV) [46]. Their LUMO levels (−1.90 to −2.18 eV) exhibit a small barrier for the electron injection from the commonly used cathode barium (−2.2 eV) [45]. Thus, these compounds might have promising potential for application in OLEDs.

Conclusion

In conclusion, six novel asymmetric 1,3,4-oxadiazole derivatives containing naphthalene and stilbene units were synthesized in good yields. The compounds exhibit a bright violet to blue emission with high fluorescence quantum yield. The absorption behaviors and emission properties depend largely on their structures. The emission behaviors of these compounds show bathochromic shifts with the increasing solvent polarity. The large Stokes shifts

(53–102 nm) and high fluorescence quantum yields (0.23–0.94) are advantages in luminous material. According to DFT calculations, these compounds possess coplanar configurations, large π conjugation, high HOMO levels (−5.70 to −5.31 eV) and wide band gaps (3.42–3.51 eV), which are beneficial for the hole-transporting or electron-transporting. Six compounds embody high HOMO levels (−5.17 to −5.03 eV) for hole injection in Cyclic voltammetry. Results show that these compounds have promising potential for the application in organic electroluminescent materials.

Acknowledgments

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.saa.2013.12.104.

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