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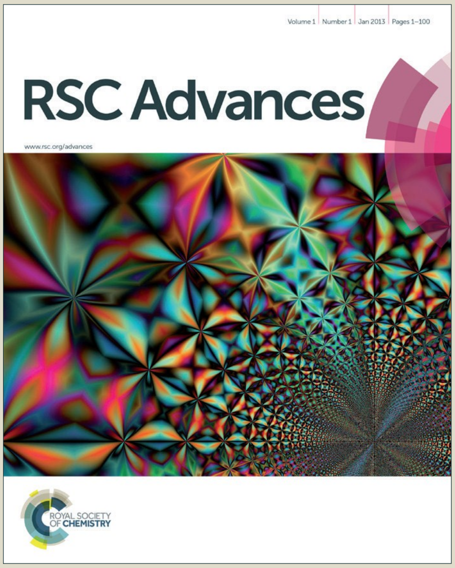

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ARTICLE

White electroluminescence from Single polymer System: Phenothiazine derivatives as red emissive dopant and Polyfluorene as blue host†

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A description of the synthesis of benzothiadiazole and phenothiazine based luminogen, 3,3'-(7,7'(benzo-1,2,5 thiadiazole-4,7-diyl)bis(10-octyl-10H-phenothiazine-7,3-diyl)bis(2-(4-bromo hexyl)acrylonitrile) (BTZPZP) that exhibit a red emission in solution as well as thin film . This monomer unit was copolymerized with 9,9-dihexyl fluorene using palladium catalysed Suzuki-cross coupling reaction where the feed ratio of the latter is varied from 0.125 to 5.0 mole % to fine tune the optoelectronic properties. White light emission is demonstrated in a copolymer BTZPZP-0.25 through incomplete energy transfer. The co-polymers of all films examined in the photoluminescence (PL) about 430 and 570-595 nm originating from fluorene segment and BTZPZP chromophore respectively. The copolymer BTZPZP-0.25 device was fabricated with (ITO/PEDOT; PSS/P(BTZPZP)s/Al) showed white electroluminiscence with Commission Internationale de l'Eclairage (CIE) coordinates of (0.32, 0.37). The maximum of current efficiency, power efficiency and brightness of the white light emitting copolymer of BTZPZP 0.25% are 4.5 cd A^{-1}, 4.2 lm W^{-1} and 9224 cd m^{-2}, respectively. The superior performance of WPLED copolymer BTZPZP-0.25 is attributed to the presence of phenothiazine group in BTZPZP monomer resulted stable electrolumenescence spectrum when the voltage level is vareid from 4V to 9V.

Introduction

Conjugated Polymers as the emissive layer in polymer light emitting diodes (PLEDs) for use in full-color flat panel displays and lighting applications.[1,2] Recently white PLEDs (WPLEDs) have also found promising application in full-color displays coupled with color filters, backlighting sources for liquid crystal displays, and solid state lighting sources.[3-6] Polyfluorene (PF) is the most promising blue light emitter for PLED applications because of its high photoluminescence quantum efficiency and good chemical and thermal stability.[7,8] The conventional white light emission based PF co-polymers for example, park et al, fabricated white light emitting diodes for single component copolyfluorene containing red emitting (0.1%) chromophore, which showed a broad emission in the entire visible region[9]. Chen et al, have reported yellow, orange and white light emitting diodes from single polymer synthesized by incorporating a small amount of 4,7-dithienylbenzotriazole into the main chain of polyfluorene.[10] Lee et al, fabricated a white phosphorent device by blending Ir(PIQ)3 with PF.[11] However, we report the white light emission significantly different electroluminescence with combination of phenothiazine and benzothiadiazole. phenothiazine is the very well-known hetero cyclic compound with electron rich sulphur and nitrogen hetero atoms, Due to that electron rich in nature, while increase the conjugation and electron with drawing nature, act as a good emitting material.[12] Nevertheless the incorporation of phenothiazine in polymeric systems was found to impart reduced hole injection barrier and balanced charge carrier mobility on white light emitting polymer.[13-16] Based on phenothiazine and other building blocks exhibited alteration of recombination zone and field dependent mobility leading to voltage dependent electroluminescence.[17-19] Benzothiadiazole has been widely investigated in constructions of various conjugated polymers showing multi-functional optoelectronic properties.[20] The reported conjugated polymers with 4,7 linkages of benzothiadiazole on the main chain were synthesized and they showed strong fluorescence in solution and thin film.[21,22]

Here in, we reported a D-A compound (BTZPZP), in which phenothiazine serves as the electron donor and Benzothiadiazole act as the electron acceptor[23]. We synthesised a series of novel random conjugated copolymers

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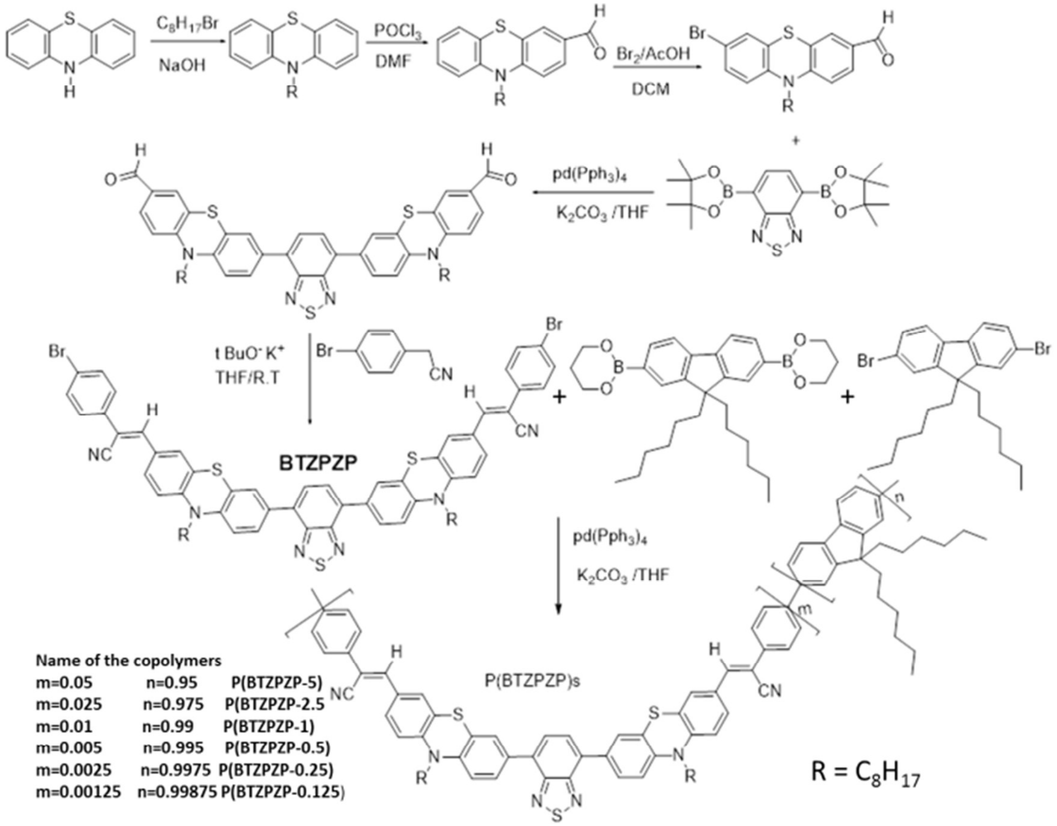
†Electronic supplementary information (ESI) available: Detailed synthetic strategy and procedure for the synthesis of monomer and copolymers H1 and C13 Spectra of monomer and H1 spectra of copolymers, computational details and GPC results.



Scheme 1 Synthetic route for monomer and copolymers with name designations

P(BTZPZP)s from dihexylfluorene and BTZPZP chromophore with high efficiency PLEDs with different colors of red and white light emissions (scheme-1). The incorporation of BTZPZP guest moiety in six energy transfer random copolymers with varying composition of (0.125 to 5.0%), which possess good absolute photo luminescence quantum yields (Φ_{PL}) and longer life time fluorescence decays in thin film. A efficient white light emission was achieved by the incorporation of very low BTZPZP content of copolymer P-BTZPZP 0.25% due to incomplete energy transfer from higher energy dihexylfluorene segments to lower energy BTZPZP moiety. Notably the device of copolymer (BTZPZP-0.25) showed no surplus long wavelength emission between EL and PL due to a significant reduction of charge trapping is attributed to the balanced charge injection. Interestingly, the Results from Atomic force microscopy revealed that formation of hallow spherical supramolecular self assemblies in all copolymers due to the formation of J-aggregates, which is supporting to the good absolute quantum yield in solid state.

Results and discussion

Synthesis and characterization of the polymers

The synthetic route and structures of the monomer and polymers are shown in scheme-1. The series of conjugated polymers were synthesized through palladium-catalyzed Suzuki coupling reactions. The actual compositions of the polymers were determined by elemental analysis. The calculated feed ratios of BTZPZP monomer in the copolymer is almost similar to experimental values are given in the supporting information. All the copolymers were found to be soluble in common organic solvents such as tetrahydrofuran(THF), chloroform and toluene with no evidence gel formation. Each copolymer was spin coated on ITO substrate and found to produce transparent and homogeneous thin films. The number average molecular weight(Mn) of the copolymers , determined by gel permeation chromatography using a polystyrene standard, were found to range from 10000 to 15000 with poly dispersity indices ranging from 2 to 3. The yields of the copolymers ranged from 69 to 78%.

Optical and photoluminescence properties

The normalized UV-vis absorption and PL emission spectra of the polymers in chloroform solution and thin film are shown in Fig 1. The absorption spectra of the monomer in solution shows the strong absorption peak at 452 nm due to intra molecular charge transfer (ICT) [24] and lower wavelength at 313nm due to π-π* transition. The absorption spectra of copolymers showed more characteristic absorption of poly (9,9-dihexylfluorene)-2,7-diyl.[25] The absorption peak for P(BTZPZP-0.125) is 373 nm due to π-π* transition of polyfluorene backbone which have low composition of BTZPZP units. The π-π* transitions of p(btzpzp-0.25),

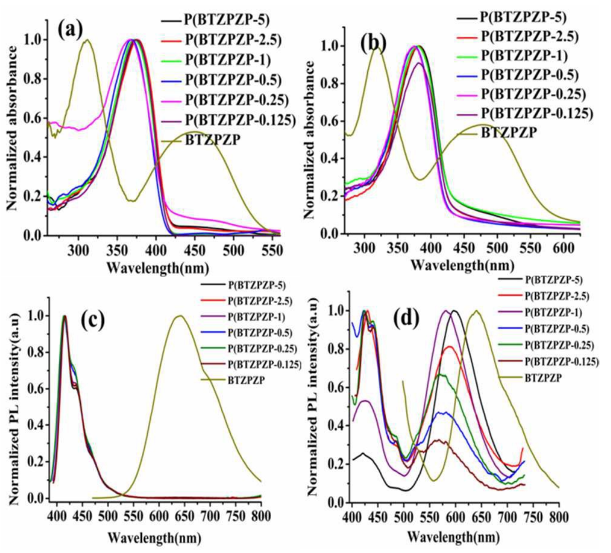


Fig 1 Absorption and PL spectra of the BTZPZP monomer and copolymers in solutions (a) and (c), in thin films (b) and (d)

p(btzpzp-0.5), p(btzpzp-1), p(btzpzp-2.5), p(btzpzp-5) copolymers were observed at 367, 368, 372, 373 and 376 nm respectively. Absorption spectra of the monomer in thin film state also shows two peaks at 334 and 502 nm which is red shifted up to 50 nm compare to solution state due to π-π stacking. Similarly the absorption bands of the all copolymers were observed at 380-389 nm in solid state and slightly red shifted was observed up to 10 nm relative to solution state absorption.

The emission spectrum of monomer in solution and thin film is 638 and 640nm respectively. In solution state, in the case of BTZPZP-5, BTZPZP-2.5 and BTZPZP-1 (highest percentage of the BTZPZP unit) exhibited two characteristic emission peaks that corresponds to the emission of poly(9,9-dihexyl fluorene)-2,7 diyl(DHFP) at 416, 415 and 415nm respectively. In addition to the above emission peaks, the BTZPZP-5, BTZPZP-2.5 and BTZPZP-1 copolymers elicited emission peaks at 632, 637 and 626nm (very low intensity) respectively, these values are closely corresponds to that of BTZPZP unit. These finding clearly indicates that there is a partial energy transfer from DHFP units to BTZPZP units. The normalized PL spectrum of the copolymers in solution and in thin film state is quite different. In thin film the copolymers exhibited two distinct emission bands at about ~430 and 570-595nm. This result indicates that the polymer chains are close packing in film states to assist inter chain energy transfer from fluorene segments to BTZPZP chromophore. The shorter wavelength (~430nm) originates from fluorene segments, while the longer wavelength can be attributed to the BTZPZP chromophore. The PL emission maxima of the copolymers shifted towards longer wavelength as the number of BTZPZP units increases in copolymers.

Life Time and Quantum Yield Studies

The fluorescence life time (τ) and quantum yield (Φ) are the most important characteristic of an organic light emitting fluorophore. To quantitatively evaluate copolymers emission, we investigated the fluorescence life time of all copolymers in chloroform solution and in thin film shown in **Fig 2**. In the solution state, the pumping wavelength all copolymers range from 367 to 373nm and probing wavelength is~415nm. All copolymers in solution state shows life time < 1ns, these unique ultrafast decay channel which was very similar to that observed in PF. These ultrafast decay channels with life time <1 ns are predominant in solution PF and P-BTZPZP copolymers[26]. In thin film the pumping wavelength of all copolymers range from 380 to 389nm and probing wavelength of all copolymers is 595, 587, 580, 580, 577 and 570nm for the composition of BTZPZP-5, 2.5, 1.0, 0.5, 0.25 and 0.125 respectively. The fluorescence life time decay in thin film is entirely different relative to solution. Notably the white light emission of copolymer BTZPZP-0.25 showed the longest life time 6.58 ns. which attributes that the highest composition of fluorenyl substituents supress the concentration quenching and increase the life time of excited state[27]. The observed lifetime of other copolymers P(BTZPZP-5), P(BTZPZP-2.5) ,P(BTZPZP-1), P(BTZPZP-0.5) and P(BTZPZP-0.125) are 4.333, 4.168, 4.353, 5.829 and 5.932 ns respectively.

The fluorescence quantum yield is the ratio of the number of photons emitted to number of photons absorbed. PL quantum yields in chloroform solution were obtained by using quinine sulphate in 0.1 H_2SO_4 (quantum yield = 0.55) as a standard. The absolute PL quantum yield in thin film was measured by using an integrating sphere. The resultant data are summarized in **Table 1.** The PL quantum yields in solution of P(BTZPZP-5), P(BTZPZP-2.5), P(BTZPZP-1), P(BTZPZP- 0.5), P(BTZPZP-0.25) and P(BTZPZP-0.125) are 0.47, 0.45, 0.63, 0.59, 0.57 and 0.60 respectively. The copolymers containing BTZPZP unit in the back bone have lower quantum yield than polyfluorene. The absolute quantum yields of copolymers BTZPZP-5, 2.5, 1.0, 0.5, 0.25, and 0.125 are 0.22, 0.14, 0.37, 0.14, 0.18 and 0.23 respectively. The quantum yield of P(BTZPZP-1) is the highest among these copolymers both in solution and thin film states, indicating that it has the optimum ratio of BTZPZP chromophore incorporation into polyfluorenes for resisting fluorescence quenching.[28]

Film morphology

The morphology of copolymers was studied using atomic force microscopy (AFM). The copolymers were found to show variation in morphology with changes in percentage composition of the BTZPZP monomer units in polymer backbone. The microscopic image revealed the circular domains with different size ranges that are clearly visible in as depicted in **Fig 3**. It is evidence from the morphological features that the composition of the BTZPZP monomer units influenced the size of the circular domains for all the copolymers in thin film.

Table 1 Spectral properties of BTZPZP monomer and copolymers**.**

Monomer/Copolymers	[a]Abs λmax(nm)		[b] Emission(nm)		[c] Lifetime(ns)		[d] Quantum yield(Φ_{PL})	
	Solution	Thin film	Solution	Thin film	Solution	Thin film	Solution	Thin film
BTZPZP	313, 452	334, 502	638	640				
BTZPZP-5	376	382	416,632	595, 430	0.689	4.333	0.47	0.22
BTZPZP- 2.5	373	389	415,637	587, 428	0.706	4.168	0.45	0.14
BTZPZP-1	372	381	415,626	580, 428	0.709	4.353	0.63	0.37
BTZPZP-0.5	368	380	413	580, 426	0.766	5.829	0.59	0.14
BTZPZP-0.25	367	380	414	577, 435	0.823	6.584	0.57	0.18
BTZPZP-0.125	373	386	416	570, 433	0.769	5.932	0.60	0.23

[a]absorption maxima in CHCl3 solutions and thin films, b emission maxima in CHCl3 solution and thin films, c fluorescence life in solutions and thin films and d quantum yield in THF solution estimated using quinine sulphate standard (error ± 0.2%) and absolute quantum yield in spun thin films in % (error ±0.4%)

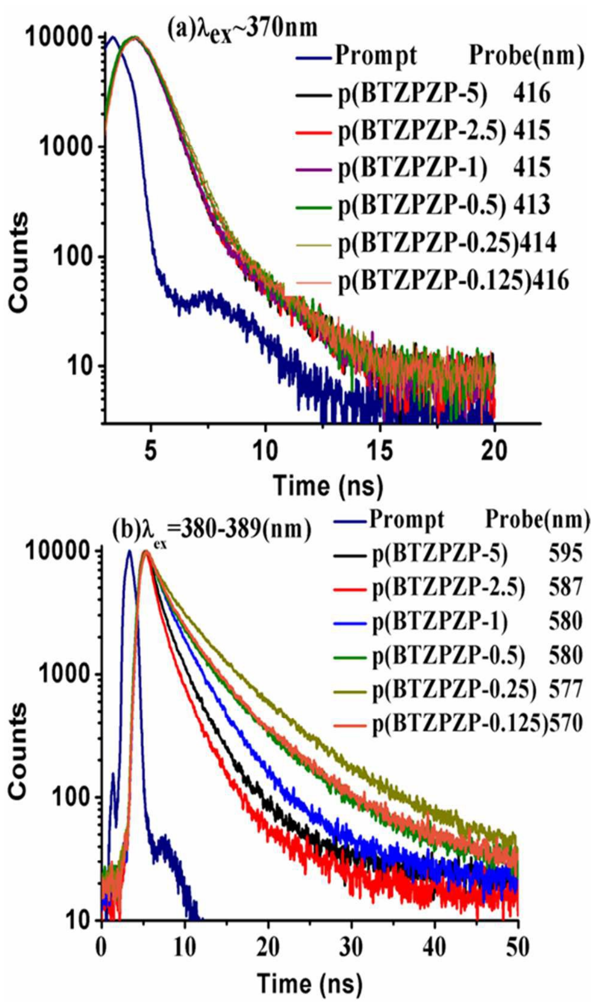


Fig 2 (a) and (b) are the fluorescence lifetime decays of the copolymers in solution and in the thin film.

The copolymer of BTZPZP-5 showed large size of circular domains with uniform size and the copolymer BTZPZP-2.5 showed a slight change in morphology with relatively to that of BTZPZP-5. It is clear from AFM micrograph that BTZPZP-1% showed a well ordered morphology where supramolecular circular domain structures are aligned normal to the surface. Because of this high ordered morphology is responsible for higher absolute quantum Yield (37.33%) of copolymer BTZPZP-1. In case the lower composition of BTZPZP-0.5, BTZPZP-0.25 and 0.125 even fewer assemblies with small radii were visible, signifying effect of BTZPZP content in the main chain of the copolymers. These findings clearly indicate the formation of hierarchical supramolecular self-assemblies of circular domains, While increasing the feed ratios of BTZPZP monomer units.[29] The red shifts appeared in the solid state may cause strong inter/intra Momolecular interactions, e.g. dipole-dipole interactions, between the polymer chains.

We have done statistical analysis for P-BTZPZP copolymers from AFM micrograph and provided in supporting information. Statistical analysis results revealed that the circular domain with different size range with small variation in morphology with change in percentage composition of the BTZPZP monomer in polymer backbone.

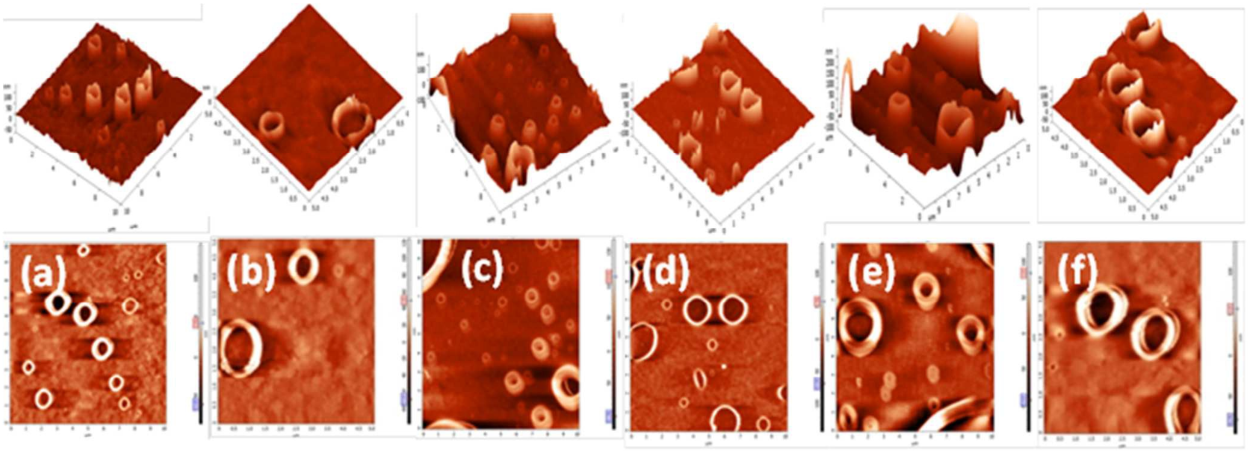


Fig 3 AFM micrographs a) P-BTZPZP-0.125, b) P-BTZPZP-0.25, C) P-BTZPZP-0.5, d) P-BTZPZP-1, e) P-BTZPZP-2.5 and f) P-BTZPZP-5.0

Electrochemical properties.

For investigating energy levels of their highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO), the electrochemical properties of copolymers, P(BTZPZP)s were investigated by cyclic voltammetry (CV). The copolymers was coated on the platinum electrode is used as the working electrode, the counter electrode was a platinum wire and the reference electrode was Ag/AgCl (0.01M) electrode. The electrochemical properties of the copolymers were investigated in an electrolyte consisting of a solution of 0.1 M Tetrabutylammoniumhexafluorophosphate in acetonitrile at the room temperature under nitrogen with a scan rate of 50 mV/s. The HOMO energy levels were calculated from onset of the oxidation potential curve according to the equation of HOMO (eV) = - (E_{ox}^{onset} + 4.82 eV) and LUMO energy levels were calculated from onset of the reduction potential curve according to the equation LUMO (eV) = - (Ered onset+ 4.8 eV) of all copolymers were estimated to be -5.82 to 6.00 eV and 3.00 to 3.20 eV, respectively. The band gaps of the all copolymers were estimated from the HOMO and LUMO levels to be 2.62 to 2.93 eV. The electrochemical band gap of all copolymers shows very little variation due to all copolymers having almost lower composition .of BTZPZP monomer .The detailed electro chemical data of these copolymers are listed in **Table 2**

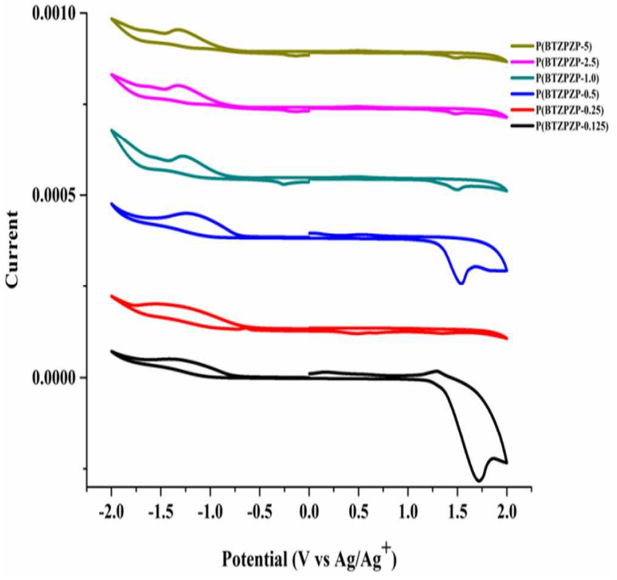


Fig 4 Cyclic voltammetry spectrum of BTZPZP copolymers

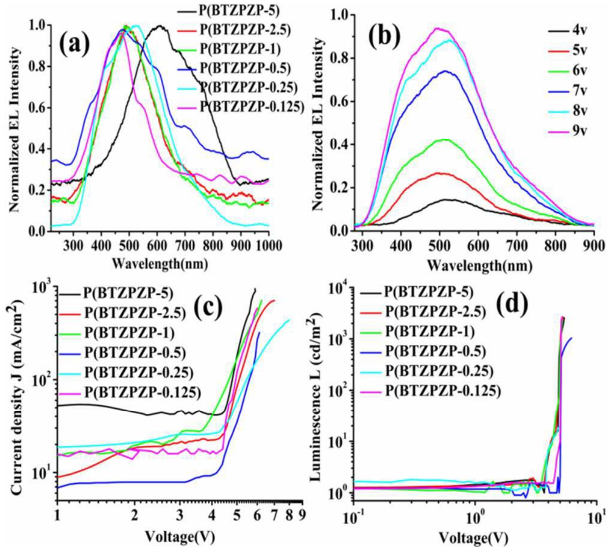


Fig 5 (a) EL spectra of BTZPZP copolymers (b) EL spectra of P(BTZPZP-0.25) in different applied voltage, (c) and (d) are current density(log scale)–voltage(log scale) (J–V) and luminescence(log)scale–voltage(log scale) (L–V) plots of OLEDs for BTZPZP copolymers

Table 2 Device characteristics of copolymers.

Polymer	^{a}HOMO (eV)	^{b}LUMO (eV)	$^cE^{ele}/E^{opt}$ (eV)	$^d\eta c^{max}$ (cd/A)	$^e\eta p^{max}$ (Lm/W)	$^fL^{max}$ (cd/m^2)	^{g}Turn-on Voltage(V)	^{h}CIE^{EL}	^{i}CIE^{PL}
P(BTZPZP-5)	-6.01	-3.16	2.85/2.87	2.9	2.3	9066.7	4.27	(0.49,0.44)	(0.47,0.39)
P(BTZPZP-2.5)	-5.82	-3.20	2.62/2.81	3.8	3.2	9248.7	4.25	(0.41,0.40)	(0.35,0.37)
P(BTZPZP-1)	-5.83	-3.15	2.68/2.83	3.3	2.9	7909.8	3.79	(0.39,0.38)	(0.39,0.41)
P(BTZPZP-0.5)	-5.93	-3.00	2.93/2.79	3.1	2.8	3656.3	3.95	(0.26,0.29)	(0.29,0.27)
P(BTZPZP-0.25)	-5.95	-3.05	2.90/2.76	4.5	4.2	9224.0	4.94	(0.32.0.37)	(0.31,0.32)
P(BTZPZP-0.125)	-5.83	-3.07	2.76/2.75	3.3	3.2	9517.2	4.41	(0.24,0.23)	(0.25,0.24)

[a] Highest Occupied Molecular Orbital, [b] Lowest Unoccupied Molecular Orbital, [C] Electrochemical band gap/Optical band gap, [d] current efficiency, [e] Power efficiency [f] Maximum brightness, [g] turn-on voltage [h] CIE coordinates for EL, [l] CIE coordinates for PL

Electroluminescence properties and current-voltage-Luminescence characteristics

To investigate the electroluminescence properties and performances of the copolymers in real devices with the configuration ITO/PEDOT:PSS/POLYMER/Al were fabricated. **Fig 5** shows the normalized EL spectra of copolymers device from BTZPZP 5 to 0.125. The EL spectra of the synthesised copolymers are different from PL spectra for lower composition due to energy transfer from higher energy state of the dihexylfluorene to low energy state of BTZPZP units in which low energy unit acts as a charge trapping sites.[30] The wavelength of EL spectra evidently increases accompanied with BTZPZP moiety gradually increase from 0.125-5 percentage. When the monomer concentration is reduced to 0.25%, device shows a balanced emission from the both host and dopant as indicated by the EL spectra as shown in **Fig 5**. From the **Fig 5a** we can see that the copolymer P(BTZPZP-0.25), emission maxima observed at 528nm related to BTZPZP monomer is slightly higher intensity than the other peak at the operating voltage of 8V. These results suggest that little more charges trapped on the BTZPZP monomer at this voltage. In addition, the narrow band gap red emitters are capable of balancing charge carrier ratio and creating Ohmic contact for hole injection, thereby improving power efficiency by decreasing power depletion.[31] The significance **d**ifference between EL and PL is attributed to the dominance of charge trapping mechanism in EL process.[32] The copolymer P(BTZPZP-0.25) device exhibited a bright white light with CIE coordinates of (0.32,0.37) exhibited a maximum luminance (Lmax) of 9224 cd/m^2 at 8V. Moreover, the EL emission spectra of P(BTZPZP-0.25) is broad covering the visible range from blue to red emission regions. The observation of electroluminescence and PL results revealed that there is no surplus long wavelength emission between electrolumescence and PL is attributed to the ambipolar charge injection. The outputs of WPLEDs were studied for their spectral ability. The OLED fabricated with BTZPZP-0.25 as an emissive layer showed a very stable spectrum with no change in relative intensity of long and shorter wavelength emissions when driving voltage from 4V to 9V as shown in **Fig 5b.** These results indicate that the use of this polymer make sure the color transparency of the EL device, which makes it of great interest for display applications. The typical voltage required to turn on and conduct current in the forward direction of the diode is defined as turn on voltage. The turn on voltage of the all copolymers, P(BTZPZP)s devices range from 3.79 to 4.94 volts and their maximum brightness are in the range from 3656-9517cd/m^2.

Theoretical study

To gain more insights into ground and excited properties, DFT calculations were performed on model systems. Optimized geometries of the model systems are shown in the SI. The calculated structures and properties of organic electronic materials in the ground and excited states with the Lee–Yang–Parr functional (B3LYP) often provide a good agreement with the experiments compared to other functionals[33-35.] Hence, all the calculation was performed by B3LYP functionals. The Computational details are given in the supporting information. The HOMO and LUMO contour plots of the model system are displayed in the **Fig 6.** It can be the seen from the **Fig 6**, the HOMO is mainly delocalized on the electron donating phenothiazine moiety and LUMO is solely concentrated on the electron withdrawing benzothiadiazole unit. From **Fig 6**, close analysis clearly reveal that there is a charge separation in the HOMOs and LUMOs. Thus, this feature confirms that there is an intramolecular charge transfer (ICT) character exhibit From phenothiazine electron donor unit to benzothiadiazole electron acceptor moiety. The calculated vertical excitation energies for monomer and dimer using TDDFT approach are listed in **Table 3**. It can be seen from the **Table 1**, the calculated spectral properties of both monomer and dimer are

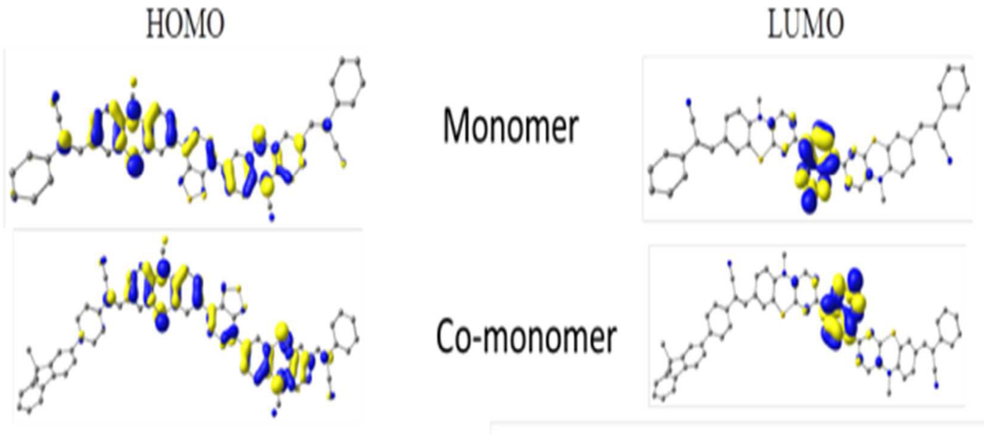


Fig 6 FMO distribution of model systems at B3LYP/6-31G* level of theory. The Hydrogen atoms omitted here for clarity.

in close agreement with experimental values. It can be seen from the **Table 1**, the calculated spectral properties of both monomer and dimer are in close agreement with experimental values. For the parent compound (BTZPZP) the ICT peak is predicted to be at 452 nm (f=0.5522) which arises from combination of HOMO to LUMO+2 and HOMO-1 to LUMO+1 transitions. Another peak is found to be at 314 nm, which is attributed as π-π* transition, which arises from combination of HOMO to LUMO+5 and HOMO-6 to LUMO transitions. In dimer, the maximum absorption peak is found to be at 431 nm (f=0.9649). For the same system, the intramolecular charge transfer peak can be seen at 574 nm (f=0.9649). This transition arises from the H-2→L+2 and H→L respectively. Emission spectra of the monomer and dimer were calculated from the optimized excited state geometries. For dimer, LUMO to HOMO transition mainly contributes to emission at 618 nm (f=0.17) which is close to the experimental value of 632 nm. However, for monomer, a significant deviation in calculated value (749 nm (f=0.15)) with respect to experimental peak (640 nm) is observed.

Conclusion

We have successfully synthesized a series of a new fluorene based copolymers P(BTZPZP)s with varying molar ratios of the narrow energy band gap monomer (BTZPZP). An efficient white light emission was achieved in a single layer polymer device by decorating BTZPZP as the red emit moiety with polyfluorene as a blue host, which exhibits good device performance in the optimized conditions. The white light emitting copolymer of P(BTZPZP-0.25) showed effective electroluminescence with CIE coordinates of (0.32, 0.37) which is close to that of standard white light emission (0.33, 0.33). The observed maximum luminance, power efficiency and current efficiency of white light emitting copolymer P(BTZPZP0.25) is 9224 cd/m2, 4.5 cd/A and 4.2 lm/W respectively. Interestingly, other copolymers exhibited all the valuable characteristics including molecular ordered supramolecular self-assembly, relatively long lifetime in aggregate state, medium turn-on voltage and very low EL operating voltage with high efficiency in device. These findings are well supported to the current study of PLEDs. The simplicity of single emissive layer polymer light emitting device architecture with high efficiency attribute to the valuable observations which makes white emitting PLEDs promising candidates for lighting applications.

Experiment details

Measurements. NMR spectra were recorded using a bruker AM 400 MHz spectrometer with tetramethylsilane as an internal reference. UV-Visible absorption spectra were recorded on Varian cary-50 Bio UV-Visible spectrometer. Photoluminescence (PL) spectra were recorded on Varian Cary eclipse fluorescence spectrometer. The number and weight average molecular weights of polymer were determined by gel permeation chromatography (GPC) on a viscotek T60A instrument, using tetrahydrofuran (THF) as eluent and polystyrene as standard. Cyclic voltammetry was done on CH instruments, CH1600D electro chemical work station with platinum working electrode by forming a thin film of the polymers on the surface of platinum working electrode. OLEDs of polymers for all devices were fabricated on glass substrates pre-coated with indium tin oxide (ITO) with sheet resistance of 10Ω per square. The substrates were cleaned with ultra-purified water, cleaned in an ultrasonic solvent bath, baked in a heating chamber of 1200C. The PEDOT-PSS (10-30nm) solution was spin coated on cleaned ITO substrates and baked in a heating chamber of 2000C for one hour. After the above process 300µl of polymer solutions with 3mg per ml concentration in CHCl3 were spin coated at 2000 rpm for 60 seconds to get uniform films of polymers (with thickness 100150nm) and Aluminium was coated at 10-5 Torr. Currentvoltage (I-V) characteristics were studied on Keithley 2400 source meter. Luminescence –voltage (L-V) characteristics of the OLEDs were studied using NUCLEONIX type 168 PMT housing with drawer assembly. Electroluminescence spectra of the OLEDs were further measured using a Carey Eclipse fluorescence spectro photometer.

Table 3 Summary of the excited state electronic transitions obtained from the TD-DFT calculations at B3LYP/6-31G* level

Compounds	solvent	States	Absorption (nm)	Energy (eV)	Oscillator strength (f)	Dominant contribution (%)[a]	Exp (nm)
BTZPZP	$CHCl_3$	S_3	462	2.68	0.5522	H→L+2(77%), H-1→L+1 (19%)	452
		S_4	459	2.69	0.2010	H→L+1(74%), H-1→ L (11%)	
		S_{18}	314	3.94	0.4039	H→L+5(162%), H-6→L (17%)	313
P(BTZPZP)	$CHCl_3$	S_1	571	2.16	0.6664	H→L (97%),	367
		S_{13}	345	3.58	0.5245	H-4→L+2 (35%), H-3→L+1 (28%)	
P(BTZPZP) (Dimer)	$CHCl_3$	S_1	574	2.16	0.9649	H→L (71%), H-1→ L (13%)	367
		S_{15}	431	2.88	0.2373	H-2→L+2 (45%), H→ L+2 (21%)	

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a H denotes HOMO and L denotes LUMO.

Materials:- Phenothiazine, Ethyl hexyl bromide, N,N-dimethyl formamide, 4-bromophenyl acetonitrile, 2,7-dibromodihexyl fluorene and 2,1,3- benzothiadiazole 4,7 diboronicester, tetrakis(triphenylphosphine)palladium(0) and 9,9dihexylfluorene-2,7-diboronic acid bis(1,3 propane diol)ester were purchased from Aldrich. Solvents with analytical grade were used during the whole experiments and all chemicals were used without further purification.

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White electroluminescence from Single Polymer System: Phenothiazine derivatives as red emissive dopant and Polyfluorene as blue host

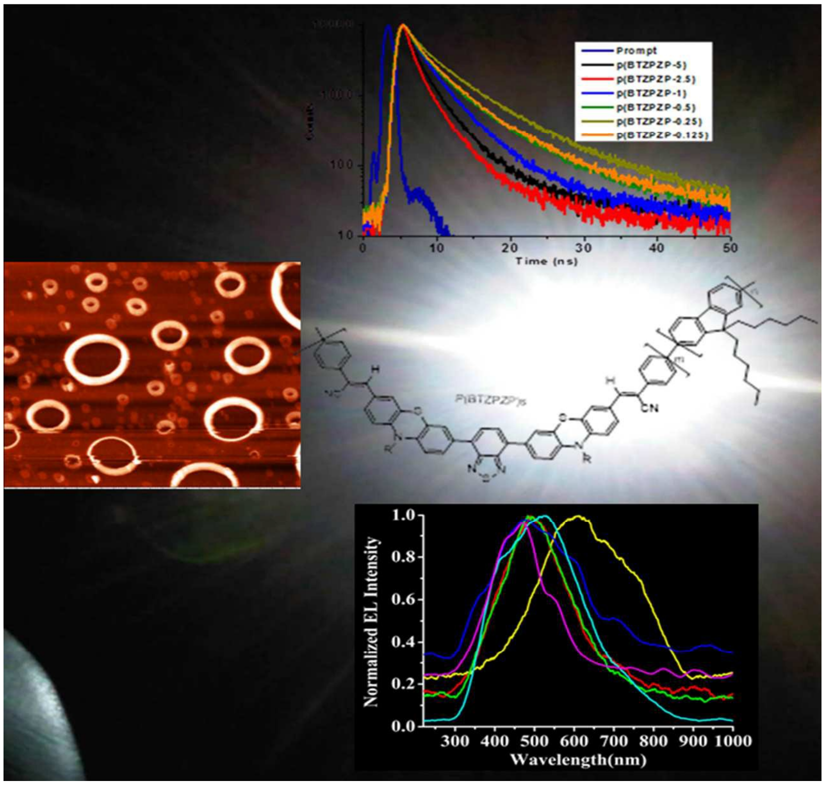

Photo physical studies of organic light emitting copolymers and their ordered supramolecular self-assembly tuning the electroluminescence properties with high efficient white light.