SUPPLEMENTARY INFORMATION

High-performance white light-emitting diodes based on Efficient Trivalent Europium molecular complex

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General Information for synthesis:

All the reactions (ligands and complexes) were completed in inert conditions. The required Solvent THF is distilled-dried by using Na Metal and benzophenone (indicator). All the commercially accessible components (Sigma Aldrich and Alpha Ezar) were cast off and deprived of extra refinement unless needed. The reaction progress was checked by thin-layer chromatography (TLC) with silica gel 60 F254 Aluminium plates (Merck) at a regular time interval. Further purification of crud, the reaction mass was carried out by the column chromatography using silica gel (Sigma-Aldrich).

Measurements:

For the structural conformation ¹H and ¹³C-NMR spectra were recorded with the help of the AV 400 Advance-III 400MHz Fourier transform nuclear magnetic resonance (FT-NMR) Spectrometer Bruker Biospin International, Switzerland. All the ¹H and ¹³C-NMR spectra were recorded in deuterated chloroform/dimethyl sulfoxide solution, and tetramethylsilane (TMS) was used as a standard reference for chemical shift measurement. The Fourier transform infrared spectroscopy (FTIR) was executed by PerkinElmer Spectrum Version 10.4.00, in the spectrum range of 400 – 4000 cm⁻¹ making KBr pellets. Mass spectra of all the synthesized

fluorophores were recorded on a High Resolution Mass Spectrometer (HRMS) Waters, USA, XEVO G2-XS QTOF model. The PL emission and excitation spectra in the solution and solid were recorded by using the Edinburg spectrofluorometric FS–5 instruments associated with SC–10 modules and SC–5 modules, respectively. The photoluminescence (excitation and emission) spectra, lifetime, and quantum yield were monitored by using Edinburg Spectrofluorometer FS–5 instruments with attaching SC – 10 modules and SC – 30 integrating sphere module. The CIE color coordinate for all emission spectra is calculated by MATLAB software.

The absorption spectra of all the synthesized compounds in solution form were UV-Visible spectrometer (Shimadzu Corporation, Japan or UV-2450 Perkin Elmer, USA/Lamda 25 and Lamda Perkin Elmer). The electrochemical properties of the ligands and their respective complex were estimated by utilizing cyclic voltammetry (CV), AUTO LAB 302N Modular potentiostat at RT in Dimethylformamide (DMF). The CV analysis is the set-up of mainly three electrodes, the working (glass-carbon rod), auxiliary (counter, Pt wire), and reference (Ag/AgCl wire) electrodes. DMF containing 0.1 M Bu₄NClO₄ was used as an electrolyte, and the sweep rate was kept at 100 mV s⁻¹. The ligand sub-atomic structures were optimized within the density functional theory (DFT) framework utilizing B3LYP/6-31G (d, p) level of theory. A UV-visible spectrum of the molecule is obtained by exciting the molecule vertically after conformation of the ground state geometry of the ligand. Further to the depiction of PL emission and excitation mechanism of the Eu(III) complex, the triplet energized condition of the ligand is additionally accessed by utilizing the same procedure specified previously. The Lifetime of the Eu(III) complex, as well as the ligand, were measured at 298 K with Edinburgh Instruments FLS 980 based on the time-correlated single-photon counting technology upon the excitation at 380 nm. A pulsed xenon lamp was used as the excitation source, and the signals were detected with a photomultiplier. All the measurements were carried out at room

temperature (RT). The G09W program effectively accomplishes the optimization study of the ligand.

Materials:

The synthesis of Eu(III) chloride(EuCl₃.6H₂O) from europium(III) oxide is done by a wellknown process. The resultant product (EuCl₃.6H₂O) was then treated with an alcoholic solution of DBM (3 eq.) in the presence of 1 N sodium hydroxide solution (3.1 eq.) to get $Eu(TTA)_3(H_2O)_2$.¹ 1,10-Phenanthroline-5,6-dione was synthesized from 1,10-phenanthroline by a previously reported procedure.²

General synthesis of ligands:

Synthesis of TPA-CHO

Triphenylamine (4.91 g, 20 mmol) was dissolved in DMF (20 mL) and placed in a 100 mL flask. Phosphorous oxychloride (10 mL) was added dropwise in the ice bath, and the reaction mixture was stirred for 10 min at 0 °C. And then, the mixture was refluxed at 80 °C for three hour under an N₂ atmosphere. Then, the reaction was quenched with cold water (300 mL), and a yellow solid was precipitated. The crude product was purified over a silica gel column with the mixture (ethyl acetate /petroleum ether, 1:50) as eluent to give TPA-CHO as a yellow solid (yield: 85%).¹H NMR (400 MHz, CDCl₃) δ (TMS, ppm): 9.80 (s, 1H), 7.67 (d, J = 8.8 Hz, 2H), 7.37–7.30 (m, 4H), 7.23–7.08 (m, 6H), 7.01 (d, J = 8.7 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ (TMS, ppm): 190.38 (s), 153.33 (s), 146.14 (s), 131.26 (s), 129.70 (s), 129.10 (s), 126.33 (s), 125.03 (s), 119.26 (s).



Synthesis of TPA-CHO-I₂

TPA-CHO (1 g, 3.66 mmol) was dissolved in acetic acid (20 mL) and placed in a 100 mL flask. KI (0.912 g, 5.495 mmol) and KIO₃ (0.783g, 3.663 mmol) was added.3 ml of H₂O was added and then the mixture was refluxed at 80 °C for 3h. Then, reaction was quenched with cold water (300 mL) and yellow solid was precipitated. The crude product was purified over a silica gel column with mixture (ethyl acetate /petroleum ether, 1:50) as eluent to give TPA-CHO-I₂ as a yellow solid (yield: 81%). ¹H NMR (400 MHz, CDCl₃) δ 9.86 (s, ¹H), 7.68 (dt, J = 30.3, 6.0 Hz, 4H), 7.70-7.51 (m, 3H), 7.28 (s, 1H), 7.15-6.99 (m, 2H), 6.91 (d, J = 8.5 Hz, 3H(I). ¹³C NMR (100 MHz, CDCl₃): δ 190.46 (s), 152.23 (s), 145.72 (s), 138.89 (s), 131.40 (s), 129.25 – 128.12 (m), 120.77 (s), 97.93 – 89.42 (m), 88.80 (s).



Synthesis of TPA-DPA-CHO

TPA-CHO-I₂ TPA-CHO (4.35g, 8.28 mmol) was dissolved in 1, 2 dichloro benzene (30mL) and placed in a 100 mL flask. Diphenyl amine/DPA (4.25 g, 2.48 mmol) and Cu powder (0.394g, 0.621 mmol), K_2CO_3 (11.43, 8.28) was added. After that (0.43g, 0.0157 mmol) mixture was refluxed at 80 °C for three hours. Then, the reaction was quenched with cold water (300 mL), and a yellow solid was precipitated. The crude product was purified over a silica gel column with the mixture (ethyl acetate /petroleum ether, 1:10 as eluent to give TPA-DPA-CHO as a yellow solid (yield: 56%).

¹H NMR (400 MHz, CDCl₃) δ 9.24 (s, 1H), 7.72 (d, J = 30.3, 6.0 Hz, 2H), 7.68 (d, J = 30.3, 6.0 Hz, 2H), 7.30 (d, 2H), 7.28 (d, 2H), 7.15 – 6.99 (m, 20H).



Synthesis of TPA-DPA-Ph:

TPA-DPA-CHO (0.725, 1.550 mmol) was added to a stirred solution of 1, 10 phenanthroline-6, 7 dione (0.325, 1.19mmol) in glacial acetic acid (30mL) at room temperature. To this reaction mixture, subsequently ammonium acetate (2.2g, 28.83mmol) and mCF₃-amine (0.122g, 1.19 mmol) was added. The resulting mixture was stirred for 12 hrs at 110°C. The progress of the reaction was monitored by TLC (MeOH in Chloroform 1:9, Rf-0.3). The RM was poured into a minimum amount of water and then added ammonium hydroxide solution. Then the formed solid was filtered and dissolved in dichloromethane, followed by drying with anhydrous sodium sulfate, and the solvent was evaporated to get a 3g crude compound. The resultant compound was purified with column chromatography by using silica gel (100-200 mesh), eluent with 5% methanol in chloroform, and the solvent was evaporated and dissolved in a minimum amount of THF solution added excess of hexane solvent, the pale yellow color solid was formed. After settling of solid, decant and repeated this process three more times and get compound 1g (63.1%) as a pale yellow solid.

¹**H-NMR Data (CDCl₃, 400MHz):**δ 9.20 (s, 1H), 9.18 (d, J = 7.7 Hz, 2H), 9.06 (s, 1H), 8.96 (d, J = 8.1 Hz, 1H), 7.71 (dd, J = 7.9, 4.5 Hz, 2H), 8.69 (d, J = 8.1 Hz, 2H), 8.64(d, J = 8.6 Hz, 1H), 8.20 (m, J = 6.3 Hz, 3H), 7.45(m, 6H), 7.2 (m, J = 7.7 Hz, 5H), 7.08 (m, J = 15.7, 8.2 Hz, 6H), 7.01(d, J = 8.8 Hz, 1H), 7.00 (d, J = 8.8 Hz, 1H).

¹³C-NMR Data (CDCl₃, 100MHz): δ 148.80, 147.98, 147.70, 138.78, 132.36, 131.29, 130.11, 129.27, 127.59, 127.08, 126.40, 126.23, 124.89, 124.25, 124.09, 123.74, 122.77, 122.77, 122.46, 119.57, 77.35, 77.24, 77.04, 76.72, 67.10 EI-MS: Exact Mass- Mass m/z 873.35 Expt.
Mass m/z = 874.55 [M + H]⁺.

Synthesis of TPA-DPA-t-Butyl:

Same procedure is followed as above for synthesis of ligand **TPA-DPA-t-Butyl**; 1, 10phenanthroline-5,6-dione (phen-dione) (1.0 g, 4.762 mmol), 3-aminobenzonitrile (0.618 g, 5.238 mmol) and 4-(trifluoromethyl)benzaldehyde (0.910 g, 5.238 mmol).

¹**H-NMR Data (400 MHz, CDCl₃):** δ 9.22 (s, 1H), 9.19 (s, 2H), 9.17 (s, 1H), 9.06 (d, J = 7.9 Hz, 1H), 8.80 (d, J = 8.0 Hz, 1H), 8.78 (d, J = 7.4 Hz, 2H), 8.68(d, J = 8.3 Hz, H), 7.50 (d, J = 9.0 Hz, 3H), 7.4 (s, 2H), 6.9 (d, J = 9.6 Hz, 7H), 2.02(9H,s)

¹³C-NMR (100 MHz, CDCl₃, TMS, δ ppm):149.65, 148.62, 138.78, 134.78, 134.22, 133.35, 132.08, 131.85, 130.67, 129.67, 127.44, 125.72, 123.88, 123.73, 122.42, 77.01, 76.70, Calculated m/z ratio = 929.12 found m/z = 930.43 [M + H]⁺.



Scheme 2: Synthetic route of ligands.

Synthesis of $Eu(TTA)_3TPA-DPA-Ph$; The solution of $Eu(TTT)_3(H_2O)_2$ (0.100 g, 0.106mol) in dry THF (15 mL) was taken in a round bottom flask and stirrer constantly unless a clear solution obtain, after 20 minutes a mixture of **TPA-DPA-Ph** (0.09 mg, 0.1062 m in dry THF was added slowly drop by drop. The reaction mixture was then stirred for 6 hours at 60°C in inert conditions. The completion of the reaction is monitored by TLC then the mixture was concentrated by a rotary evaporator and then dissolved in the least amount of THF.To this solution, excess hexane was added by the wall of the round bottom flask; the residue was obtained. The upper solvent layer was then decanted slowly, and the residue was dried. The same procedure was repeated several times to achieve the final complex in pure powder form.found: $\mathbf{m/z} = 1755.26 [M + 2Na^++H_2O^+]^+$.

Synthesis of $Eu(TTA)_3TPA-DPA-t-Butyl$; The complex was synthesized by previously described procedure using TPA-DPA-t-Butyl as the ligand instead of ligand1. ESI-MS: m/z = 1748.66 [M + 1Na⁺+3K⁺]⁺.

Synthesis of yellow organic dye

Aldehyde (1.831 mmol, 1 eq.) and NaOH (1.831 mmol, 1 eq.) were added to a mixture of 30 mL of water and 25 mL of ethanol, then 1-phenylethanone (3.663 mmol, 2 eq.) was added. The mixture was heated and stirred at 90°C for four hour. After cooling, the mixture was filtered and washed with plenty of water and then dried at RT to produce a yellow powder with a yield of 80%, and the synthetic scheme-3 for the preparation of the yellow dye is shown below.⁴



Scheme 3. Synthesis of TPA substituted yellow organic dye.

1. NMR Spectroscopy:



Fig S1. ¹H NMR spectroscopy of TPA-CHO



Fig S2. ¹H NMR spectroscopy of TPA-CHO-I₂ in CDCl_{3.}



Fig S3. ¹H NMR spectroscopy of TPA-DPA-CHO in CDCl_{3.}



Fig S4. ¹H NMR spectroscopy of TPA-DPA-Ph in CDCl₃



Fig S5. ¹H NMR spectroscopy of TPA-DPA-t-Butyl in CDCl₃

2. Mass spectral analysis:



Figure S6. Mass spectral data of TPA-DPA-Ph



Figure S7. Mass spectral data of TPA-DPA-t-Butyl



Fig S8. Mass spectral data of Eu(TTA)₃TPA-DPA-Ph



Fig S9. Mass spectral data of Eu(TTA)₃TPA-DPA-t-Butyl

PL spectra:





Fig S10. Different excitation spectral wavelength analysis of the Eu (TTA)₃TPA-DPA-Ph and

Eu(TTA)₃TPA-DPA-t-Butyl complex in solid-state.

 Table ST1.The Infrared frequencies (wavenumber in cm⁻¹) for free ligand and its corresponding Eu(III)-complexes.

Complex	v (C=O)	ν (C=N)	ν (C=C)	v (C-F)	v (Eu-N)	v (Eu-O)
Eu (TTA) ₃ TPA-	1602	1588	1408	1135	577	464
DPA-Ph						
Eu (TTA) ₃ TPA-	1606	1563	1411	1139	580	467
DPA-t-Butyl						
TPA-DPA-Ph	-	1482	1383	1120	-	-
TPA-DPA-t-Butyl	-	1493	1376	1122	-	-

Eu(TTA) ₃ -TP	Eu(TTA)3-TPA-DPA-Ph		Eu(TTA) ₃ -TPA	A-DPA-t-Butyl
X	y		X	y
0.6625	0.3326	Toluene	0.6311	0.3282
0.6763	0.3340	CHCl ₃	0.6663	0.3340
0.5898	0.3379	THF	0.5257	0.3262
0.6341	0.3219	DCM	0.6630	0.3261
0.6660	0.3361	DMSO	0.6634	0.3366
0.6669	0.3394	DMF	0.6610	0.3250
0.6579	0.3368	ACN	0.5663	0.3161

Table ST2. The calculated CIE from the PL emission data of Eu(III) complexes in different solvents .

Table ST3. Intensity ratios and CIE color coordinates for the Eu (III) Complexes in different

 concentration ratios doped PMMA.

%	Eu(T)	[A) ₃ -TPA-]	DPA-Ph	Color	Eu(TTA) ₃ -TPA-DPA-T-Butyl		Color Purity	
	I ₂ / I ₁		CIE	Purity	I ₂ /I ₁	CIE		-
		x	У			x	у	-
1:99	15.81	0.6673	0.3369	91.71	16.03	0.6490	0.3291	92.16
2:98	15.83	0.6663	0.3305	93.83	16.21	0.6480	0.3290	93.92
3:97	15.69	0.6646	0.3322	94.57	16.02	0.6430	0.3211	94.95
4:96	15.84	0.6641	0.3323	95.07	16.69	0.6430	0.3280	93.57

Sl. No.	Compound name	Volatage _{oxi} onset[V] (E _{HOMO} [eV])	Volatage _{red} ^{onset} [V] (E _{HOMO} [eV])	λ _{onset} d [nm]	Energy gap [eV]
1	TPA-DPA-Ph	1.79 (-6.19)	-1.11(-3.29)	426	2.91
2	Eu(TTA) ₃ -TPA-DPA-Ph	1.23 (-5.63)	-1.32(-3.08)	386	2.55
3	TPA-DPA-t-Butyl	1.38(-5.78)	-1.53(-2.87)	417	2.91
4	Eu(TTA)3- TPA-DPA-t- Butyl	1.32(-5.72)	-1.21(-3.08)	495	2.64

Table ST4. Electrochemical properties of the ligands and respective Eu(III)-complexes.

 Table ST5. Experimental Lifetime data of ligands and complexes in solid-state.

Complex/ Ligands Name	Solid(ns/ms)
TPA-DPA-Ph	1.54 ns
TPA-DPA-t-Butyl	0.69 ns
Eu(TTA) ₃ -TPA-DPA- Ph	0.554 ms
Eu(TTA) ₃ -TPA-DPA- t-Butyl	0.699 ms

PLQY:



Fig S11. The photoluminescence quantum yield of Eu(TTA)₃-TPA-DPA- Ph



Fig S12. The photoluminescence quantum yield of Eu(TTA)₃-TPA-DPA- t-Butyl

Judd-Ofelt (J –O) analysis:

The Judd-Ofelt parameters investigation of the emission spectrum is a potent tool for calculating the parity forbidden electric-dipole radiative transition rates between the different levels of the lanthanide ions. To study the chemical environment impact on the luminescent characteristics of the Eu³⁺ ions, it is probable to analyze the Ω_{λ} ($\lambda = 2, 4, 6$) parameters from the emission spectra by the standard calculation method. The experimental intensity parameters were calculated for the ${}^{5}\text{D}_{0} \rightarrow {}^{7}\text{F}_{2}$ and ${}^{5}\text{D}_{0} \rightarrow {}^{7}\text{F}_{4}$ transitions by maintaining ${}^{5}\text{D}_{0} \rightarrow {}^{7}\text{F}_{1}$ transition as a reference, and the detailed calculation are given in our previous reports.^{3, 4} The following equation explains the relationship between the radiative emission rate and integrated emission intensity.

$$\frac{A_{0-2,4}}{A_{0-1}} = \frac{I_{0-2,4} h \vartheta_{0-1}}{I_{0-1} h \vartheta_{0-2,4}}....(1)$$

Where I_{0-J} is the area under the spectral curve and hv_{0-J} is the energy related to the ${}^{5}D_{0} \rightarrow {}^{7}F_{J}$ (J = 1, 2, 4) transition of Eu³⁺. The magnetic dipole radiative (${}^{5}D_{0} - {}^{7}F_{2}$) transition rate A_{0-1} was considered as 50s⁻¹. The above relation was given the probability of the electric dipole transition. The forced electric dipole transitions ${}^{5}D_{0} \rightarrow {}^{7}F_{2}$ and ${}^{5}D_{0} \rightarrow {}^{7}F_{4}$ as a function of Judd– Ofelt intensity parameter are expressed as

Where v is the Lorentz local field correction factor which is a function of refractive index n=2.02 of the host and is given by the relation $\chi = n (n^{2}+9)^{2/9}$. $\langle {}^{5}D_{0} | U_{J} | {}^{7}F_{2} \rangle^{2}$ are the square reduced matrix elements, independent of the chemical environment of the Eu³⁺ ion. The values of non-zero square reduced matrix $\langle {}^{5}D_{0} | U_{J} | {}^{7}F_{2} \rangle^{2} = 0.0032$ for ${}^{5}D_{0} \rightarrow {}^{7}F_{2}$ transition and $\langle {}^{5}D_{0} | U_{J} | {}^{7}F_{4} \rangle^{2} = 0.0023$ for ${}^{5}D_{0} \rightarrow {}^{7}F_{4}$ transition were taken for the present calculations. The Ω_{2} values are much higher than the Ω_{4} , which indicates the ${}^{5}D_{0} \rightarrow {}^{7}F_{2}$ transition is dominating. Ω_{2} parameter shows dependence on the covalence between rare-earth cations and ligand field anions which reveal about local environment of Eu³⁺ site and its asymmetry. Hence, it is highly sensitive to the ligand environment, which can be seen by the adjustments in its value with increasing Eu³⁺ ion concentration. The higher Ω_{2} value signifies higher asymmetry or high covalence nature of Eu³⁺ ions and ligand bonds in the current host lattice. The change of Ω_{2} parameter was observed due to distortions present around occupied Eu³⁺ ion site.

To understand further, the overall quantum yield (Φ_{Tot}) (Eqn. 3) was calculated and other lifetime parameters also been calculated for Eu^{III} complexes. The $\Phi_{overall}$ obtained under ligand excitation and it depends on two essential parameters. The primary one, the efficiency of energy transfer from the ligand to the Eu^{III} ion (Φ_{sens}), and another one is the intrinsic quantum yield (Φ upon direct excitation into the f level).

The intrinsic quantum yield (Φ_{Ln}) of the Eu³⁺ ion can calculate with τ_{obs} and τ_{rad} life time, the equation (4) followed as

$$\Phi_{\rm Ln} = \frac{(\frac{A_{RAD}}{A_{RAD} + A_{NR}})}{\tau_{RAD}} = \frac{\tau_{obs}}{\tau_{RAD}}.....(4)$$

The radiative lifetime (τ_{RAD}) can be calculated by corrected emission spectrum according to using equation 5. It is assuming that the energy of the ${}^5D_0 \rightarrow {}^7F_1$ transition (MD) and its oscillator strength are constant. Here, I_{TOT}/I_{MD} is the ratio of the total area of the corrected Eu³⁺ emission spectrum to the area of the ${}^5D_0 \rightarrow {}^7F_1$ band, $A_{MD,0}$ (14.65 s⁻¹) represents the spontaneous emission probability of the ${}^5D_0 \rightarrow {}^7F_1$ transition (in vacuo), and n is the refractive index of the medium. An average index of refraction (1.5) was employed in the calculation.^{1,2,3}

$$A_{RAD} = \frac{\left(\frac{1}{\tau_{RAD}}\right)}{\tau_{RAD}} = A_{MD,0}n^3 \left(\frac{I_{TOT}}{I_{MD}}\right).$$
(5)

From the relative areas of the ${}^{5}D_{0}-{}^{7}F_{J}$ emission transitions (which associates with the already predicted J–O theory) of Eu³⁺ ion is used to determine the experimental branching ratio (β_{1-3}). In general, the efficiency of the energy transfer from the ligand to Eu^{III} ion can be predicated by the obtained intrinsic quantum yield (Φ_{Ln}) and energy transfer efficiency (η_{sens}). Here, the photosensitized energy transfer process is explained by using a simple schematic diagram (Fig. 12 in main text). First, the organic ligand in the lanthanide(III) complex is excited by photoirradiation at the π - π * transition band, and then, a T₁ state of the ligand is formed. The energy transfer process between the T₁ and 4f–4f transition bands of the Eu-ion (4f–4f') is generally explained by the Förster and Dexter mechanisms. Effective energy transfer (forward energy transfer) between the T₁ (donor) and 4f–4f' (acceptor) leads to the formation of an excited Ln(III) complex. However, a small energy gap between the T₁ state and emitting level of the Ln(III) ion promotes energy back transfer from the 4f–4f' emitting level (donor) to the T₁ state (acceptor), resulting in the prevention of effective forward energy transfer. Thus, effective energy transfer is dependent on the energy gap between the T_1 state and the emitting level in Eu(III) complexes.⁶



77K spectra of ancillary ligands

Fig S13. Phosphorescence spectra of TPA-DPA-Ph and TPA-DPA-t-Butyl at 77K.

LED Fabrication process:

LED is based on using ultraviolet (UV) LED chip and a phosphor that absorbs the UV or violet light and converts it to a white light. Due to its similarity to conventional fluorescent lamps [4], this approach has been proposed multiple times prior to the advent of GaN-based blue LEDs. A near UV LED (NUV) chip was coated with two distinct dopant concentrations of PMMA:Eu(III) complexes to produce the intense red LEDs. Phosphor is dissolved with THF and stirred

Table ST6 Ra, LER and R9 values of three component and two component LEDs.

Name of the	R9	R1	R2	R3	R4	R5	R6	R 7	R8	Ra	LER
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compound											
(93%)-											
Eu(TTA) ₃ -	65	89	91	91	88	89	88	90	86	89	230
TPA-DPA-Ph											
(87%)											
Eu(TTA) ₃ - TPA-DPA-Ph	19	84	89	97	86	84	88	94	73	89.25	284

DFT Analysis:



Fig S14 Ground state optimized structure of ligands

Table ST6 Optimized geometry of ligands and their frontier molecular orbital pictures.

Ligands	НОМО	LUMO	HOMO-1	LUMO+1
TPA-DPA-m-CN		A Contraction of the second se		





Fig S15. UV spectrum from DFT in the gas phase.

Device fabrication

The europium complex dissolved in THF solvent. A suitable host material (PMMA) is added to the complex solution. This can be done by dissolving the complex in a polymer solution and casting it onto a substrate or embedding it in a sol-gel matrix. A gel type host -complex substance is prepared at string both PMMA and complex mixture in THF at room temperature. The gel is prepared with 1:10 and 1:50 w/W ratio. The LED device is constructed by depositing the luminescent layer (gel substance) onto a LED chip. Spin coating is also followed to make the LED chip solvent and moisture-free. Spin coating method is applied to a small amount of gel onto the LED and spin it at a controlled speed to achieve an even layer. Near UV LED (NUV) chip was coated with two distinct dopant concentrations of PMMA:Eu(III) complexes to produce the intense red LEDs. LEDs will work only if they are forward-biased; hence, it is essential to identify the electrodes accurately before installing them into a circuit. The combination of red phosphor and yellow phosphor on a blue LED (InGaN chip) generated hybrid WLEDs. With accurate concentration (x10⁻⁶), yellow organic dye (reported organic molecule) is employed with Eu(TTA)₃TPA-DPA-Ph (as a red phosphor) at 1µm dissolved in PMMA gel (in THF). The mix should cover the full visible spectrum. The organic dye was responsible for the yellow area in the WLED spectrum. The white LEDs are fabricated by integrating the red and yellow phosphors into a single device. Typically, this involves creating a white light by combining emissions from the two phosphors using a single blue LED chip.







Fig S15. DSC curve of complexes showing $T_{\rm g}$.

Table ST7 The computed vertical transitions and there oscillator strengths (f) and configuration of the ligands.

Luminophores	State	Energy (eV)	λ _{max} nm	f	Configuration
TPA-DPA-mCN	Gas	2.298	539.3	0.016	HOMO→LUMO (69.95%)
Singlet		2.871	431.8	0.024	HOMO-1→LUMO (65.94%)
		2.872	431.6	0.131	HOMO-1 \rightarrow LUMO (21.44%)
Triplet	Gas	2.274	545.0	0	$HOMO \rightarrow LUMO + 1 (63.89\%)$ $HOMO \rightarrow LUMO (68.25\%)$ $HOMO - 2 \rightarrow LUMO (11.35\%)$
		2.508	494.2	0	HOMO-2→LUMO+1 (20.73%) HOMO→LUMO+1(37.58%)
		2.794	443.6	0	HOMO-1→LUMO (12.36%) HOMO→LUMO+6 (51.43%)
TPA-DPA-pCN Singlet	Gas	2.308	537.0	0.019	HOMO-2→LUMO (10.17%) HOMO→LUMO (69.80%)
		2.868	432.2	0.003	HOMO-1→LUMO (69.20%)
		2.931	423.0	0.089	HOMO-2→LUMO+1 (10.21%) HOMO→LUMO+1 (66.21%)
Triplet	Gas	2.274	545.0	0	HOMO-2→LUMO (13.96%) HOMO→LUMO (66.87%)

		2.527	490.4	0	HOMO-2→LUMO+2 (27.49%)
					HOMO→LUMO (18.80%)
					HOMO→LUMO+2 (50.43%)
		2.798	443.0	0	HOMO-1→LUMO (13.29%)
					HOMO-1→LUMO+4 (10.79%)
					HOMO-1→LUMO+11 (15.47%)
					HOMO→LUMO+5 (33.62%)
TPA-DPA-Ph	Gas	3.022	410.2	0.760	HOMO→LUMO (67.84%)
Singlet		3.144	394.2	0.003	HOMO-2→LUMO+1 (13.55%)
					HOMO→LUMO (11.13%)
					HOMO→LUMO+1 (67.17%)
		3.277	378.2	0.054	HOMO→LUMO+2 (25.03%)
					HOMO \rightarrow LUMO+ (50.43%)
Triplet	Gas	2.514	492.9	0	HOMO-2→LUMO (29.37%)
					HOMO→LUMO (54.21%)
					HOMO→LUMO+2 (13.16%)
					HOMO→LUMO+5 (12.78%)
		2.781	445.7	0	HOMO-1→LUMO (11.44%)
					HOMO→LUMO+5 (26.53%)
					HOMO→LUMO+6 (48.82%)
		2.867	432.3	0	HOMO-2→LUMO (30.30%)
					HOMO→LUMO+11 (13.72%)
TPA-DPA-t-	Gas	3.024	409.8	0.785	HOMO→LUMO (66.54%)
Butyl					HOMO→LUMO+1 (17.13%)
Singlet		3.167	391.4	0.008	HOMO-2→LUMO+1 (13.09%)
					HOMO→LUMO+1 (65.96%)
		3.264	379.8	0.0692	HOMO→LUMO+2 (40.37%)
					HOMO→LUMO+3 (51.03%)
					HOMO→LUMO+6 (10.87%)
Triplet	Gas	2.512	493.5	0	HOMO-2→LUMO (27.64%)
					HOMO-2→LUMO+1 (12.03%)
					HOMO→LUMO (52.21%)
					HOMO→LUMO (21.12%)
		2.769	445.69	0	HOMO-1→LUMO (10.64%)
					HOMO-1→LUMO+11 (14.43%)
					HOMO→LUMO+2 (12.00%)
					HOMO→LUMO+3 (19.96%)
					HOMO→LUMO+5 (50.74%)
		2.868	432.2	0	HOMO-4→LUMO+ (11.58%)
					HOMO-2→LUMO (28.34%)
					HOMO-2→LUMO+1 (18.53%)

Table ST8. xyz coordinates of ligands

TPA-DPA- mCN

6 9.536052000 1.631568000 -0.082854000

6	8.191128000	1.329860000	-0.103813000
6	7.775903000	-0.017816000	-0.139060000
6	8.802952000	-1.018101000	-0.121022000
6	10.459699000	0.577065000	-0.095427000
6	6.418087000	-0.483062000	-0.164426000
6	8.460708000	-2.447173000	-0.100170000
6	7.100927000	-2.846851000	-0.080680000
6	6.092142000	-1.830331000	-0.108133000
6	6.802573000	-4.220144000	-0.043402000
1	5.765573000	-4.533005000	-0.029899000
6	7.842252000	-5.123871000	-0.029781000
6	9.158938000	-4.629867000	-0.055528000
1	9.876390000	2.659971000	-0.052705000
1	7.463637000	2.127831000	-0.084283000
1	11.527523000	0.781716000	-0.087653000
1	7.661677000	-6.192101000	-0.002187000
1	9.998169000	-5.321539000	-0.048620000
6	4.199986000	-0.814102000	-0.153813000
7	4.736999000	-2.015272000	-0.096526000
7	5.185587000	0.178085000	-0.202154000
6	2.750024000	-0.588654000	-0.139993000
6	2.100126000	0.478722000	-0.777840000
6	1.947056000	-1.541178000	0.511372000
6	0.718293000	0.598236000	-0.755266000
1	2.665549000	1.212759000	-1.335066000
6	0.569356000	-1.421480000	0.548535000
1	2.430506000	-2.377728000	0.999239000
6	-0.078068000	-0.344163000	-0.084121000
1	0.246243000	1.422636000	-1.273849000
7	10.109350000	-0.696616000	-0.107535000
7	9.466715000	-3.345155000	-0.088935000
1	-0.018082000	-2.161843000	1.076023000

6	-2.094881000	1.067249000	-0.079894000
6	-3.155788000	1.327947000	-0.954990000
6	-1.671344000	2.090440000	0.777397000
6	-3.783623000	2.566094000	-0.963647000
1	-3.502765000	0.545101000	-1.618765000
6	-2.273833000	3.340607000	0.744393000
1	-0.853070000	1.907823000	1.463641000
6	-3.347741000	3.598612000	-0.120627000
1	-4.612208000	2.742028000	-1.638363000
1	-1.924056000	4.121519000	1.408195000
6	-2.312830000	-1.373064000	-0.007375000
6	-3.381977000	-1.445310000	0.893459000
6	-2.099406000	-2.450177000	-0.876537000
6	-4.219355000	-2.552195000	0.916116000
1	-3.567268000	-0.617140000	1.566915000
6	-2.914524000	-3.572711000	-0.830609000
1	-1.277625000	-2.413441000	-1.581653000
6	-3.995239000	-3.640300000	0.060571000
1	-5.048581000	-2.583427000	1.612107000
1	-2.724521000	-4.400594000	-1.502536000
6	4.971044000	1.591166000	-0.221289000
6	5.175209000	2.311760000	-1.400167000
6	4.548889000	2.238705000	0.934934000
6	4.958323000	3.686789000	-1.419759000
1	5.501503000	1.788735000	-2.291081000
1	4.392416000	1.674751000	1.845073000
6	4.530494000	4.346763000	-0.272887000
1	5.118400000	4.244917000	-2.334279000
1	4.354664000	5.414930000	-0.282415000
7	-1.478381000	-0.218032000	-0.050229000
7	-4.840651000	-4.778912000	0.093197000
7	-3.978986000	4.868363000	-0.137379000

6	-5.288196000	-5.298968000	1.337987000
6	-6.615188000	-5.722122000	1.496832000
6	-4.411129000	-5.397215000	2.427160000
6	-7.047290000	-6.238201000	2.714158000
1	-7.301918000	-5.645522000	0.662746000
6	-4.857033000	-5.898431000	3.645735000
1	-3.382038000	-5.079231000	2.312741000
6	-6.174796000	-6.326056000	3.797480000
1	-8.077362000	-6.560693000	2.818632000
1	-4.164264000	-5.967511000	4.477177000
1	-6.516758000	-6.722285000	4.746379000
6	-5.243176000	-5.399082000	-1.121076000
6	-5.252537000	-6.795840000	-1.238289000
6	-5.635424000	-4.623908000	-2.220984000
6	-5.652735000	-7.398255000	-2.426503000
1	-4.946490000	-7.402722000	-0.394888000
6	-6.017607000	-5.234852000	-3.410845000
1	-5.638185000	-3.543978000	-2.136637000
6	-6.033064000	-6.624112000	-3.521408000
1	-5.653290000	-8.480191000	-2.499706000
1	-6.318453000	-4.619551000	-4.251631000
1	-6.337466000	-7.096933000	-4.447760000
6	-4.214947000	5.562860000	1.081766000
6	-4.698954000	4.883892000	2.208003000
6	-3.965901000	6.938816000	1.173883000
6	-4.918829000	5.567513000	3.399473000
1	-4.899670000	3.821413000	2.143412000
6	-4.205183000	7.617562000	2.364213000
1	-3.585796000	7.469732000	0.309631000
6	-4.678254000	6.937653000	3.485162000
1	-5.293291000	5.026736000	4.261580000
1	-4.006018000	8.682100000	2.418509000

1	-4.855842000	7.468153000	4.413236000
6	-4.396522000	5.442863000	-1.368571000
6	-3.569131000	5.388381000	-2.498795000
6	-5.643756000	6.074036000	-1.472354000
6	-3.987236000	5.943620000	-3.703707000
1	-2.600600000	4.908826000	-2.426139000
6	-6.046189000	6.641719000	-2.676831000
1	-6.291595000	6.117359000	-0.605419000
6	-5.225007000	6.577117000	-3.801109000
1	-3.333965000	5.892074000	-4.567823000
1	-7.014745000	7.125502000	-2.738577000
1	-5.544825000	7.014335000	-4.739668000
6	3.879811000	4.293357000	2.092094000
6	4.322974000	3.621201000	0.908334000
7	3.520937000	4.839110000	3.044350000
ТР	A-DPA- pCN		
6	-9.567366000	1.316232000	-0.102651000
6	-8.214099000	1.055459000	-0.073805000
6	-7.758260000	-0.278481000	-0.020533000
6	-8.754680000	-1.309430000	-0.029708000
6			
6	-10.458770000	0.234526000	-0.080166000
U	-10.458770000 -6.387020000	0.234526000 -0.702160000	-0.080166000 0.015324000
6	-10.458770000 -6.387020000 -8.369580000	0.234526000 -0.702160000 -2.727654000	-0.080166000 0.015324000 -0.031730000
6 6	-10.458770000 -6.387020000 -8.369580000 -6.998283000	0.234526000 -0.702160000 -2.727654000 -3.086367000	-0.080166000 0.015324000 -0.031730000 -0.041712000
6 6 6	-10.458770000 -6.387020000 -8.369580000 -6.998283000 -6.020537000	0.234526000 -0.702160000 -2.727654000 -3.086367000 -2.039673000	-0.080166000 0.015324000 -0.031730000 -0.041712000 -0.023874000
6 6 6 6	-10.458770000 -6.387020000 -8.369580000 -6.998283000 -6.020537000 -6.658796000	0.234526000 -0.702160000 -2.727654000 -3.086367000 -2.039673000 -4.450416000	-0.080166000 0.015324000 -0.031730000 -0.041712000 -0.023874000 -0.060721000
6 6 6 6 1	-10.458770000 -6.387020000 -8.369580000 -6.998283000 -6.020537000 -6.658796000 -5.612888000	0.234526000 -0.702160000 -2.727654000 -3.086367000 -2.039673000 -4.450416000 -4.732335000	-0.080166000 0.015324000 -0.031730000 -0.041712000 -0.023874000 -0.060721000 -0.066680000
6 6 6 6 1 6	-10.458770000 -6.387020000 -8.369580000 -6.998283000 -6.020537000 -6.658796000 -5.612888000 -7.670757000	0.234526000 -0.702160000 -2.727654000 -3.086367000 -2.039673000 -4.450416000 -4.732335000 -5.385170000	-0.080166000 0.015324000 -0.031730000 -0.041712000 -0.023874000 -0.060721000 -0.066680000 -0.066309000
6 6 6 1 6 6	-10.458770000 -6.387020000 -8.369580000 -6.998283000 -6.020537000 -6.658796000 -5.612888000 -7.670757000 -9.001774000	0.234526000 -0.702160000 -2.727654000 -3.086367000 -2.039673000 -4.450416000 -4.732335000 -5.385170000 -4.930842000	-0.080166000 0.015324000 -0.031730000 -0.041712000 -0.023874000 -0.060721000 -0.066680000 -0.066309000 -0.051345000
6 6 6 1 6 6 1	-10.458770000 -6.387020000 -8.369580000 -6.998283000 -6.020537000 -6.658796000 -5.612888000 -7.670757000 -9.001774000 -9.938231000	0.234526000 -0.702160000 -2.727654000 -3.086367000 -2.039673000 -4.450416000 -4.732335000 -5.385170000 -4.930842000 2.333551000	-0.080166000 0.015324000 -0.031730000 -0.041712000 -0.023874000 -0.060721000 -0.066680000 -0.066309000 -0.051345000 -0.145322000
6 6 6 1 6 1 6 1 1	-10.458770000 -6.387020000 -8.369580000 -6.998283000 -6.020537000 -6.658796000 -5.612888000 -7.670757000 -9.001774000 -9.938231000 -7.511316000	0.234526000 -0.702160000 -2.727654000 -3.086367000 -2.039673000 -4.450416000 -4.732335000 -4.732335000 -4.930842000 2.333551000 1.875033000	-0.080166000 0.015324000 -0.031730000 -0.041712000 -0.023874000 -0.060721000 -0.066680000 -0.066309000 -0.051345000 -0.145322000 -0.100014000

1	-7.457939000	-6.447725000	-0.079509000
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6	-2.102449000	0.400438000	0.620766000
6	-1.880667000	-1.649210000	-0.609949000
6	-0.723701000	0.553938000	0.613967000
1	-2.692795000	1.135128000	1.150446000
6	-0.505884000	-1.496975000	-0.630118000
1	-2.336246000	-2.510769000	-1.080813000
6	0.105776000	-0.388125000	-0.016339000
1	-0.280168000	1.403943000	1.116195000
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7	-9.348039000	-3.655610000	-0.035287000
1	0.107246000	-2.237336000	-1.127691000
6	2.084494000	1.072921000	-0.015840000
6	3.082437000	1.399200000	0.909380000
6	1.686056000	2.046460000	-0.939766000
6	3.674983000	2.654710000	0.903018000
1	3.407294000	0.654036000	1.625715000
6	2.254221000	3.312962000	-0.926902000
1	0.914570000	1.810086000	-1.663009000
6	3.265780000	3.636936000	-0.010566000
1	4.454062000	2.884821000	1.619251000
1	1.927042000	4.056632000	-1.642951000
6	2.369213000	-1.361152000	-0.020797000
6	3.471523000	-1.417008000	-0.882293000
6	2.157102000	-2.429357000	0.859949000
6	4.341401000	-2.498363000	-0.855400000
1	3.656763000	-0.595221000	-1.563536000

6	3.005933000	-3.527643000	0.862461000
1	1.310605000	-2.405366000	1.535686000
6	4.118885000	-3.578157000	0.010787000
1	5.195507000	-2.516465000	-1.521139000
1	2.816884000	-4.349157000	1.542444000
6	-5.004274000	1.414949000	0.041617000
6	-5.241181000	2.147525000	1.207197000
6	-4.595587000	2.061189000	-1.124887000
6	-5.071808000	3.525019000	1.207396000
1	-5.556099000	1.631758000	2.106107000
1	-4.416361000	1.480748000	-2.020964000
1	-5.253506000	4.099018000	2.107232000
7	1.502884000	-0.229697000	-0.028056000
7	4.997656000	-4.691831000	0.027240000
7	3.860957000	4.923745000	-0.009715000
6	5.498920000	-5.221953000	-1.192494000
6	6.841171000	-5.611640000	-1.301080000
6	4.660445000	-5.363544000	-2.307001000
6	7.325809000	-6.137746000	-2.494053000
1	7.498162000	-5.501608000	-0.447063000
6	5.158474000	-5.874697000	-3.501013000
1	3.620256000	-5.071317000	-2.231019000
6	6.491333000	-6.269091000	-3.602668000
1	8.366896000	-6.434075000	-2.559655000
1	4.494925000	-5.977861000	-4.352525000
1	6.874157000	-6.673317000	-4.532400000
6	5.378143000	-5.277217000	1.265720000
6	5.423647000	-6.670649000	1.410642000
6	5.712036000	-4.470337000	2.362051000
6	5.802737000	-7.238620000	2.622510000
1	5.162214000	-7.301978000	0.570180000
6	6.073221000	-5.047320000	3.575185000

1	5.685853000	-3.392564000	2.256593000
6	6.125408000	-6.433216000	3.713367000
1	5.831923000	-8.318504000	2.717061000
1	6.328757000	-4.407784000	4.412859000
1	6.413417000	-6.879434000	4.657969000
6	4.168111000	5.568308000	-1.239500000
6	4.747902000	4.851344000	-2.295006000
6	3.897090000	6.932318000	-1.413694000
6	5.039930000	5.485777000	-3.498105000
1	4.968075000	3.798675000	-2.165479000
6	4.208284000	7.562099000	-2.614291000
1	3.444199000	7.492285000	-0.604677000
6	4.776941000	6.844301000	-3.665113000
1	5.489630000	4.916355000	-4.304045000
1	3.991247000	8.617955000	-2.732222000
1	5.012065000	7.336907000	-4.601276000
6	4.156967000	5.570851000	1.221662000
6	3.233357000	5.553481000	2.275564000
6	5.376702000	6.237842000	1.399332000
6	3.529830000	6.183229000	3.479980000
1	2.285274000	5.046599000	2.143430000
6	5.657693000	6.879041000	2.601421000
1	6.097764000	6.252442000	0.591224000
6	4.740227000	6.853098000	3.650278000
1	2.802836000	6.161894000	4.284302000
1	6.606049000	7.390946000	2.721802000
1	4.964974000	7.348786000	4.587361000
6	-4.419125000	3.438645000	-1.129025000
1	-4.101350000	3.946395000	-2.030818000
6	-4.477808000	5.598605000	0.035537000
6	-4.657240000	4.178939000	0.037304000
7	-4.333244000	6.744429000	0.035178000

TPA-DPA-t-butyl

6	9.407124000	0.500270000	-0.031791000
6	8.040198000	0.321805000	-0.039208000
6	7.505164000	-0.981671000	0.031461000
6	8.436816000	-2.066900000	0.128106000
6	10.231190000	-0.630897000	0.048426000
6	6.110026000	-1.321084000	0.034131000
6	7.965578000	-3.454650000	0.240496000
6	6.574529000	-3.728063000	0.267515000
6	5.662357000	-2.627990000	0.168639000
6	6.153378000	-5.064049000	0.385566000
1	5.092141000	-5.280540000	0.405094000
6	7.106528000	-6.055406000	0.469023000
6	8.462602000	-5.684629000	0.431597000
1	9.839872000	1.492524000	-0.084548000
1	7.385137000	1.178615000	-0.094530000
1	11.313325000	-0.523284000	0.051301000
1	6.829318000	-7.099246000	0.559940000
1	9.235724000	-6.447132000	0.493888000
6	3.876512000	-1.441120000	0.049870000
7	4.297265000	-2.684910000	0.181495000
7	4.947904000	-0.552060000	-0.051280000
6	2.450468000	-1.090052000	0.044596000
6	1.900811000	0.032996000	-0.591556000
6	1.561677000	-1.975030000	0.680725000
6	0.532351000	0.264690000	-0.587201000
1	2.533101000	0.725943000	-1.127760000
6	0.197775000	-1.741755000	0.700189000
1	1.968618000	-2.850898000	1.169077000
6	-0.347374000	-0.612911000	0.063990000
1	0.137315000	1.129469000	-1.104938000
7	9.767417000	-1.865264000	0.129364000

7	8.885647000	-4.437397000	0.322449000
1	-0.457443000	-2.433527000	1.214374000
6	-2.241895000	0.957897000	0.088993000
6	-3.273238000	1.340608000	-0.777985000
6	-1.731103000	1.912946000	0.977809000
6	-3.786542000	2.630224000	-0.748232000
1	-3.685541000	0.613871000	-1.467488000
6	-2.219584000	3.212226000	0.983186000
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SI-35

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