Electronic Supplementary Information

A Unique White Electroluminescent One-Dimensional Europium(III) Coordination Polymer

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Content

Table S1. Crystal data and structure refinement of **Eu-FDPO**.

Formula	C94 H69 Eu O8 P2
Formula weight	1540.39
T (K)	293(2)
Crystal system	Monoclinic
Space group	C 2/C
a (Å)	52.7880(17)
b (Å)	12.4054(3)
c (Å)	25.0467(8)
β (deg)	113.292(4)
V ($Å^3$)	15065.3(8)
Z	8
ρ (g/cm^3)	
μ (mm^{-1})	1.358
F(000)	6320
crystal size (mm)	0.30 × 0.25 × 0.21
θ (deg)	3.06 to 26.00
Index ranges	$-64 \leq h \leq 60$
	$-15 \leq k \leq 15$
	$-28 \leq l \leq 30$
Absorption correction	Multi-scan
Max. and min. transmission	0.8279 and 0.7668
GOF on F2	1.056
R1, R2 [I > 2σ (I)]	0.0367, 0.0771
R1, R2 (all data)	0.0620, 0.0853
Largest diff. peak and hole ($e.Å^{-3}$)	0.811 and -0.709

Table S2. Selected bond lengths (Å) and angles (degree) of **Eu-FDPO**.

Bond length (Å)			
Eu1-O3	2.341(2)	P1-O4	1.485(2)
Eu1-O8	2.3468(19)	P1-C72	1.791(3)
Eu1-O4	2.3627(18)	P1-C78	1.793(3)
Eu1-O7	2.364(2)	P1-C61	1.794(3)
Eu1-O1	2.3858(19)	P2-O2	1.4817(18)
Eu1-O2	2.4148(18)	P2-C75	1.793(3)
Eu1-O6	2.448(2)	P2-C76	1.797(3)
Eu1-O5	2.451(2)	P2-C85	1.803(3)

Bond angle (°)			
O3-Eu1-O8	104.52(8)	O3-Eu1-O5	81.22(8)
O3-Eu1-O4	146.32(7)	O8-Eu1-O5	68.63(7)
O8-Eu1-O4	88.51(8)	O4-Eu1-O5	74.81(7)
O3-Eu1-O7	94.85(8)	O7-Eu1-O5	144.68(7)
O8-Eu1-O7	144.72(8)	O1-Eu1-O5	71.14(7)
O4-Eu1-O7	91.39(7)	O2-Eu1-O5	125.87(7)
O3-Eu1-O1	71.63(7)	O6-Eu1-O5	131.46(7)
O8-Eu1-O1	139.66(7)	O4-P1-C72	114.07(14)
O4-Eu1-O1	78.35(7)	O4-P1-C78	110.10(13)
O7-Eu1-O1	74.32(7)	C72-P1-C78	106.75(14)
O3-Eu1-O2	71.72(7)	O4-P1-C61	110.99(13)
O8-Eu1-O2	74.04(7)	C72-P1-C61	105.95(14)
O4-Eu1-O2	141.90(7)	C78-P1-C61	108.73(14)
O7-Eu1-O2	84.79(7)	O2-P2-C75	112.30(12)
O1-Eu1-O2	135.65(7)	O2-P2-C76A	112.38(12)
O3-Eu1-O6	141.18(7)	C75-P2-C76A	110.08(13)
O8-Eu1-O6	76.34(7)	O2-P2-C85	108.73(13)
O4-Eu1-O6	71.69(7)	C75-P2-C85	105.57(13)
O7-Eu1-O6	70.21(7)	C76A-P2-C85	107.43(13)
O1-Eu1-O6	132.23(7)	C73-C83-C69	110.9(2)
O2-Eu1-O6	71.38(7)		

Table S3. Physical properties of **Eu-FDPO**.

Absorption (nm)	Emission (nm)	PLQY[c] (%)
227, 260, 287, 311, 347[a]	580, 593, 613, 656, 706[a]	24[a]
246, 304, 364[b]	579, 592, 612, 655, 702[b]	85[b]
S_1/T_1 (eV)	HOMO/LUMO (eV)	μ_e/μ_h[g] (10^{-7} cm^2 V^{-1} s^{-1})
3.07[d]/-	-5.5[f]/-2.6[f]	5.4/0.79
3.78[e]/2.42[e]	-4.851[e]/-1.068[e]	

[a] In CH_2Cl_2 (10^{-5} mol L^{-1}); [b] in film; [c] calculated by using $Ru(bpy)_3Cl_2$ as standard; [d] estimated according to the absorption edges; [e] DFT calculated results of pendamer; [f] calculated according to the equation HOMO/LUMO = -4.78 - onset voltage of redox peaks; [g] estimated according trap-free space charge limited current model.

Particle Size Distribution of Eu-FDPO in DMSO Solution

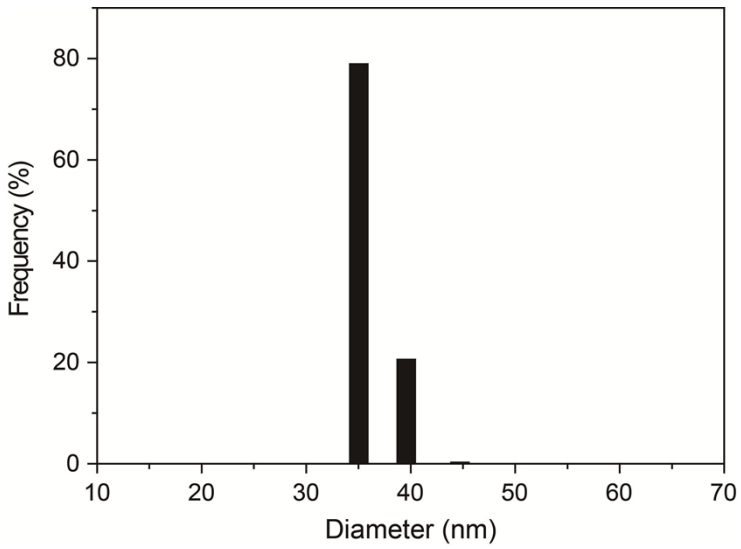

Figure S1. Particle size distribution of dilute DMSO solutions of **Eu-FDPO** (10^{-1} g L^{-1}) measured by dynamic light scattering technology.

DFT Calculation Results of Eu-FDPO

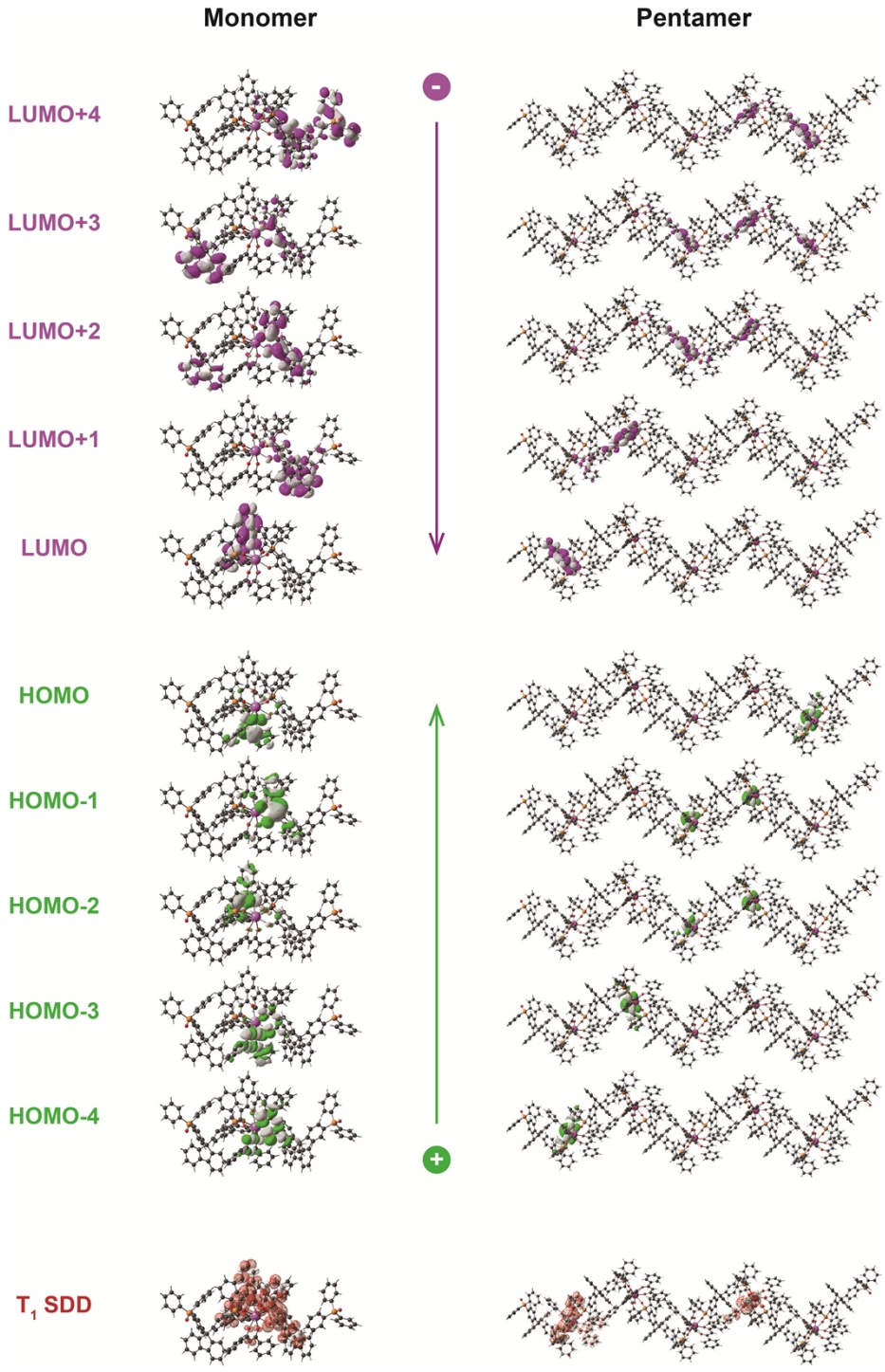

Figure S2. Contours of FMOs and T_1 SDD of monomer and pentamer of **Eu-FDPO** by DFT simulation.

Electrical Properties of Eu-FDPO

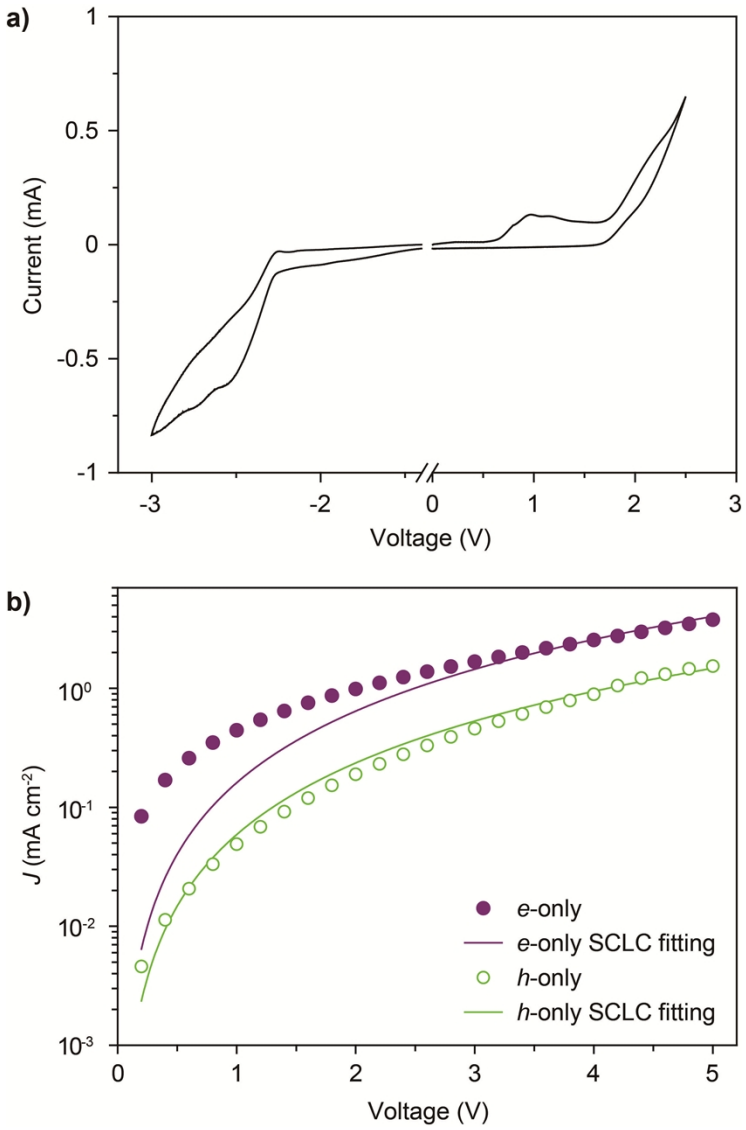

Figure S3. a) Cyclic voltammogram of **Eu-FDPO**. The measurement was performed in THF and dichloromethane for reduction and oxidation, respectively, with tetrabutylammonium hexafluorophosphate as electrolyte and a silver/silver nitrate (Ag/Ag^{+}) reference electrode at room temperature in nitrogen at a scanning rate of 100 mV s^{-1}; b) *I-V* characteristics of nominal single-carrier transporting devices based on **Eu-FDPO** and the corresponding fitting curves by SCLC model.

Table S4. EL performance of representative Eu^{3+} metallopolymers.

Ref.	Polymer Type	Device	Voltage (V)[a]	L_{Max} (cd m^{-2})	Maximum efficiencies[b]	Efficiency roll-offs (%)[c]			CIE coordinate
						CE	PE	EQE	
[1]	Wolf-I	PEDOT:PSS/Eu^{3+} polymer:PBD/Ba	12.5, 13.5, 15.5	149	0.41, 0.09, 0.43	26	33	26	0.67, 0.33
[2]	Wolf-I	PEDOT:PSS/PVK/Eu^{3+} polymer:OXD-7/Ba	17, -, -	68	0.18, 0.03, 0.37	-	-	-	-, -
[3]	Wolf-I	Eu^{3+} polymer/LiF/Ca:Ag	8, 15, 18	126	0.56, -, -	-	-	-	-
[4]	Wolf-I	PEDOT:PSS/Eu^{3+} polymer/BCP/Alq_3/LiF/Al	17, -, -	42	<0.5, 0.035, -	-	-	-	0.66, 0.33
[5]	Wolf-I	PVK/Eu^{3+} polymer/Ba	15, 25, -	11	-, -, 0.07	-	-	-	-, -
This work	Wolf-III	PEDOT:PSS/PVK:PBD:**Eu-FDPO**/Ca (**I**)	8.8, -, -	7	0.01, 0.003, 0.01	-	-	-	0.46, 0.33
This work	Wolf-III	PEDOT:PSS/PVK:PBD:**Eu-FDPO**/B3PYMPM/Ca (**II**)	7.6, 8.4, 10.2	215	0.71, 0.27, 0.37	38	52	38	0.38, 0.32
This work	Wolf-III	PEDOT:PSS/PVK:**FDPO**:**Eu-FDPO**/B3PYMPM/Ca (**III**)	12.5, 13.9, 15.9	240	0.22, 0.05, 0.14	18	20	21	0.28, 0.29

[a] In the order of onset, 10 and 100 cd m^{-2}; [b] in the order of CE (cd A^{-1}), PE (lm W^{-1}) and EQE (%); [c] at 100 cd m^{-2}.

References

[1] H. Xu, R. Zhu, P. Zhao and W. Huang, *J. Phys. Chem. C* **2011**, *115*, 15627-15638.

[2] C. Yang, J. Xu, Y. Zhang, Y. Li, J. Zheng, L. Liang and M. Lu, *J. Mater. Chem. C* **2013**, *1*, 4885-4901.

[3] Q. D. Ling, Q. J. Cai, E. T. Kang, K. G. Neoh, F. R. Zhu and W. Huang, *J. Mater. Chem.* **2004**, *14*, 2741-2748.

[4] Z.-G. Zhang, J.-B. Yuan, H.-J. Tang, H. Tang, L.-N. Wang and K.-L. Zhang, *J. Polym. Sci. A* **2009**, *47*, 210-221.

[5] J. Pei, X.-L. Liu, W.-L. Yu, Y.-H. Lai, Y.-H. Niu and Y. Cao, *Macromolecules* **2002**, *35*, 7274-7280.