Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Red Emissive Organic Light-Emitting Diodes based on Codeposited Inexpensive Cu^{I} Complex

Tianchi Ni,[a] Xiaochen Liu,[a] Tao Zhang,[b] Hongliang Bao,[c] Ge Zhan,[a] Nan Jiang,[b] Jianqiang Wang,[c*] Zhiwei Liu,[a*] Zuqiang Bian,[a] Zhenghong Lu,[b] and Chunhui Huang[a]

[a]Beijing National Laboratory for Molecular Sciences (BNLMS), State Key Laboratory of Rare Earth Materials Chemistry and Applications, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, P. R. China

[b]Department of Physics, Yunnan University, 2 Cuihu Bei Lu, Kunming, 650091, P. R. China.

[c]Key Laboratory of Interfacial Physics and Technology ,Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201204, P. R. China.

E-mails: zwliu@pku.edu.cn, wangjianqiang@sinap.ac.cn

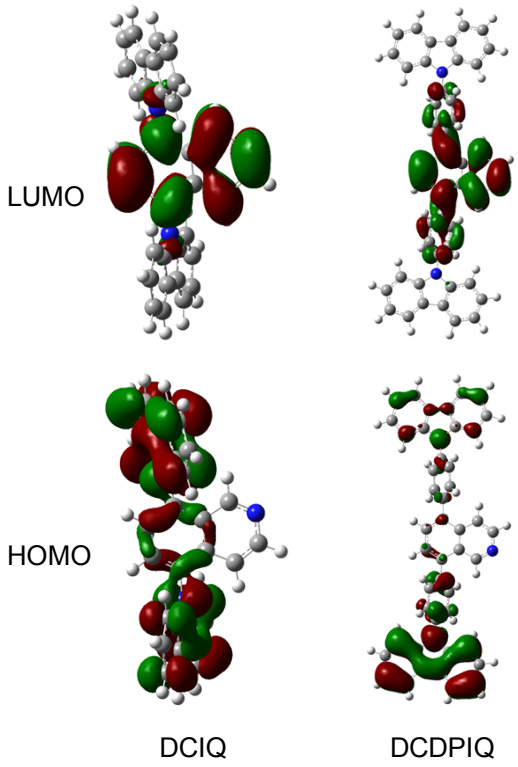

Fig. S1. DFT calculations of the spatial distributions of the HOMO and LUMO level for DCIQ and DCDPIQ.

Table S1. DFT calculated energy levels of DCIQ and DCDPIQ.

Compound	HOMO-1 [eV]	HOMO [eV]	LUMO [eV]	LUMO+1 [eV]	E_g [eV]	T_1-S_0 [eV]	T_2-S_0 [eV]
DCIQ	6.22	6.05	2.25	1.54	3.80	2.36	2.95
DCDPIQ	5.94	5.85	2.27	1.45	3.58	2.27	2.96

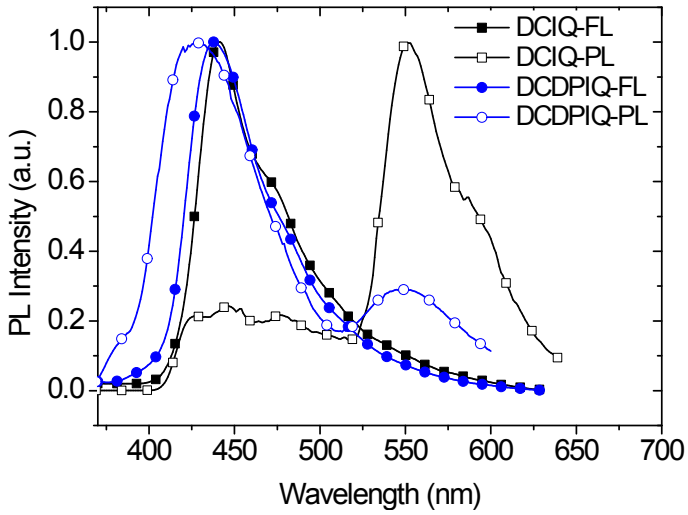

Fig. S2. Fluorescence (FL) and phosphorescence (PL) spectra of DCIQ and DCDPIQ in solid state.

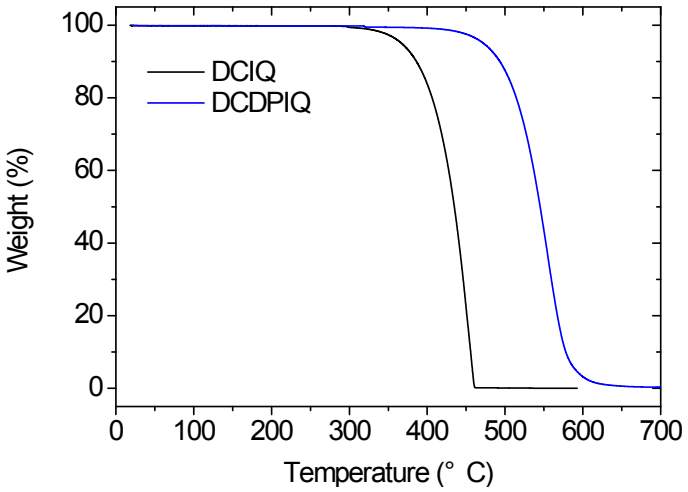

Fig. S3. TGA thermograms of DCIQ and DCDPIQ recorded at a heating rate of 15 °C min^{-1}.

Table S2. Photophysical properties of codeposited CuI:CIQ (CIQ = DCIQ, DCDPIQ) films with different CuI:CIQ molar ratios.

CuI:CIQ molar ratio	DCIQ		DCDPIQ	
	λ_{em} [nm]	PLQY [%]	λ_{em} [nm]	PLQY [%]
1:3	631	19	621	15
1:5	631	24	621	12
1:7	631	16	617	14
1:9	631	16	615	14
1:11	627	15	618	13

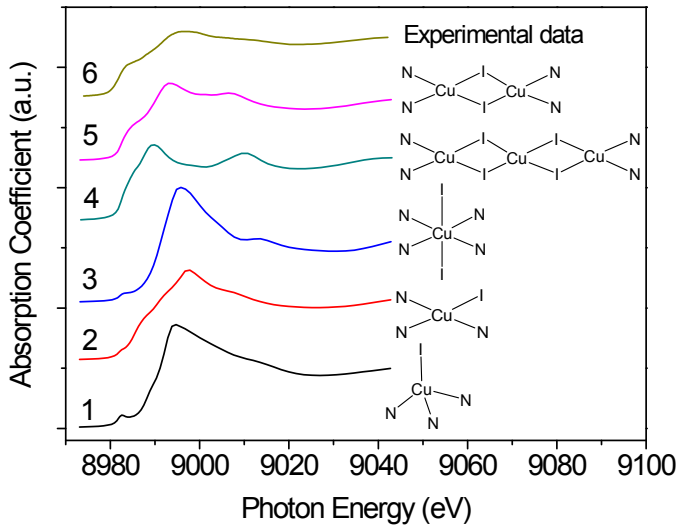

Fig. S4. Experimental data (curve 6) and calculated data (curves 1-5) for Cu *K*-edge XANES of the codeposited CuI:DCDPIQ film with corresponding local structure model on the right.

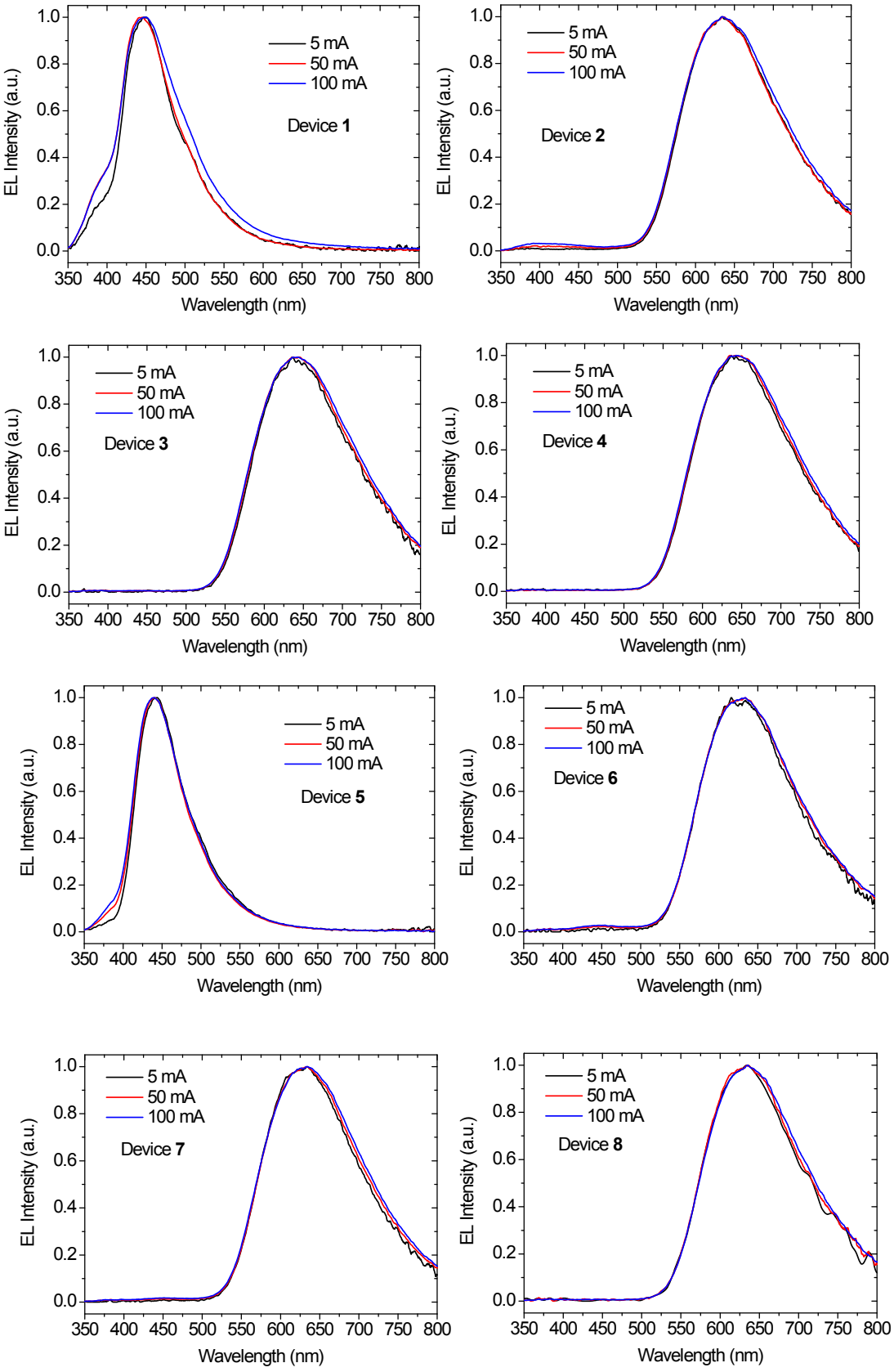

Fig. S5. EL spectra of devices **1**-**8** at different currents.