

## Electronic Supplementary Material (ESI)

For

### Soft salts from dinuclear cationic and mononuclear anionic iridium (III) complexes for OLEDs devices

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## A- Experimental details

### A-1-Materials and physical measurements:

– All reagents and solvents were purchased from Aldrich or Alfa Aesar and used as received without further purification. Dimer  $\text{Ir}_2(\text{dfppy})_4\mu\text{-Cl}_2^{1,2}$  (dfppy = 2-(2',4'-difluorophenyl pyridine) were synthesized in a inert atmosphere according to the Nonoyama route by refluxing  $\text{IrCl}_3 \cdot 3\text{H}_2\text{O}$  with 2–2.5 equiv. of cyclometalating ligand in a 3:1 mixture of 2-ethoxyethanol and water. Heteroleptic complex  $\text{NBu}_4[\text{Ir}(\text{dfppy})_2(\text{NCS})_2]^{3,4}$  (**NBu<sub>4</sub>.A**) was synthesized from procedures adapted from the literature with tetrabutylammonium thiocyanate. ESI-HRMS measurements were carried out with a Waters Xevo-QTOF.

– <sup>1</sup>H spectra were recorded at room temperature in 5 mm o.d. tubes on a Bruker Avance 300 spectrometer equipped with a QNP probe head. - Elemental analyses were performed by the "Service central d'analyse du CNRS", Gif-sur-Yvette (France).

– U.V.-visible absorption spectra were recorded on a Varian CARY 5000 spectrophotometer with scale ranging from 200 to 800 nm or 250 to 800 nm depending of the solvent, in transmission mode. Spectrophotometric grade solvents were used. The fluorescence excitation spectra were recorded using a FluoroMax3 (Jobin Yvon Horiba) and emission was corrected for the spectral sensitivity of the instrument. The fluorescence quantum yield was calculated using  $[\text{Ru}(\text{bpy})_3]\cdot\text{Cl}_2$  as reference (0.54). The absorbance of the solutions used to determine the fluorescence quantum yields did not exceed 0.1 at the excitation wavelength.

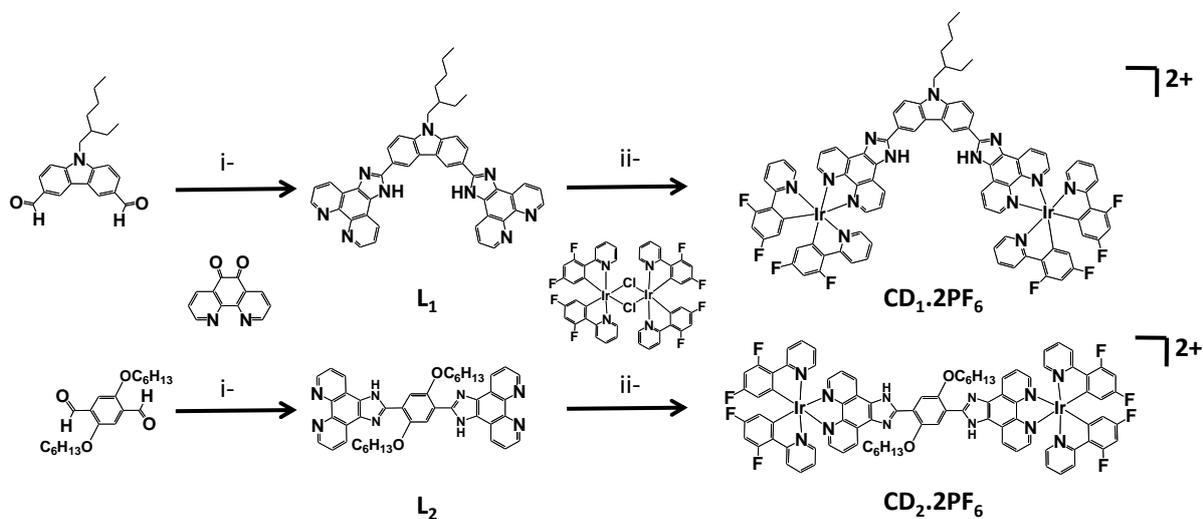
– Electrochemical measurements were performed in a three electrode cell equipped with a 1 mm diameter platinum disk as the working electrode, carbon rod as the counter electrode and  $\text{Ag}^+$  (0.01 M)/Ag as the reference electrode. The reference potential was checked vs. ferrocene as recommended by IUPAC ( $E^\circ(\text{Fc}) = + 86 \text{ mV}$ ).<sup>5</sup> The supporting electrolyte was tetrabutylammonium hexafluorophosphate (Fluka, puriss.) and the solutions were deaerated by argon bubbling prior to each experiment. Cyclic voltammograms (CVs) were recorded with a 600 CH Instruments potentiostat connected to a PC.

– Solid state spectroscopic data were obtained on thin films of material deposited by sublimation under secondary vacuum ( $10^{-6}$  mbar) from organic-designed temperature-controlled thermal oven with alumina beds. Thickness of approx. 50 nm was controlled using

built-in piezoelectric sensor assuming a material density of 1.25. Solid state absorption and emission spectra were recorded with a UV MC2 spectrophotometer from the SAFAS Monaco society and a Photon Technology International spectrofluorimeter.

– All theoretical calculations were performed using the Gaussian03 program<sup>6</sup> in vacuum on a Nec TX7 with 32 processors Itanium 2 of the MESO center of the ENS Cachan. Orbitals were generated with the cubgen module of Gaussian and visualized with GaussView 3.0 of Gaussian Inc. GaussSum 2.1 was used for the electronic spectrum simulation. The equation employed by the program to calculate the theoretical spectrum and the extinction coefficients is based on Gaussian convolution and is reported in the open source code of the program (available at <http://gausssum.svn.sf.net/viewvc/gausssum/Trunk/src/gausssum/>).

**Computational method:** All calculations were carried out using the Gaussian code.<sup>7</sup> The hybrid Hartree–Fock/density functional model B3LYP was used for geometry optimization and orbitals generation and the hybrid PBE0 model one for TDDFT. The 6-31+G(d) basis set was used for all calculations on ligand and a mixed basis set for the complexes namely double  $\zeta$  quality LANL2 and corresponding pseudo-potential for the metal and 6-31+G(d) for all other atoms. Such a level of theory was proven to provide reliable results both for thermochemical and spectroscopic properties.<sup>8</sup> No symmetry constraints were applied and, in the case of oxidized systems, unrestricted calculations were performed and spin contamination, monitored by the S2 expectation value, was found to be negligible. Counteranions or counterocations were not taken into account. When referring to spin density, Mulliken spin distributions are considered.



**Scheme SI-1.** Synthetic route for the preparation of **CD<sub>1</sub>.2PF<sub>6</sub>** and **CD<sub>2</sub>.2PF<sub>6</sub>**. i- NH<sub>4</sub>OAc, CH<sub>3</sub>COOH, ii- CHCl<sub>3</sub>/EtOH, NH<sub>4</sub>PF<sub>6</sub>

**2-(9-(2-ethylhexyl)-3-(1H-imidazo[4,5-f][1,10]phenanthroline-2-yl)-9H-carbazol-6-yl)-1H-imidazo[4,5-f][1,10]phenanthroline (L<sub>1</sub>).**

9-(2-Ethylhexyl)carbazole-3,6-dicarboxaldehyde (170 mg, 0.507 mmol) was suspended in 30 mL of acetic acid. After dissolution at refluxed (110°C), ammonium acetate (1.8 g, 18.3 mmol) and 1,10-phenanthroline-5,6-dione (230 mg, 1.09 mmol) were added to the solution and the resulting mixture was stirred at reflux overnight. After evaporation of the solvent under reduced pressure, a solid precipitated after addition of methanol (30 mL). The solid L<sub>1</sub>

was filtered off and washed with water, EtOH, dried with ether and under vacuum. Yield: 126 mg (35%). HR-ESI-MS ( $m/z$ ): 716.3167 [ $L_1-H$ ]<sup>+</sup> (716.3172, theor.). <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz),  $\delta$  = 9.25 (s, 2H), 9.15-8.95 (m, 8H), 8.45 (d, 2H), 7.86 (m, 4H), 7.75 (d, 2H), 4.31 (m, 2H), 1.51-1.12 (m, 9H), 0.9 (t, 3H, *J* = 8.0 Hz), 0.8 (t, 3H, *J* = 8.0 Hz). Anal. Calcd for C<sub>46</sub>H<sub>37</sub>N<sub>9</sub> : C, 77.18; H 5.21; N, 17.61. Found: C, 77.54; H, 5.43; N, 17.93.

**2-(2,5-bis(hexyloxy)-4-(1H-imidazo[4,5-f][1,10]phenanthroline-2-yl)phenyl)-1H-imidazo[4,5-f][1,10]phenanthroline (L<sub>2</sub>).** 1,10-phenanthroline-5,6-dione (126 mg, 0.6 mmol) and ammonium acetate (1380 mg, 17.9 mmol) were added to a solution of 2,5-bis(hexyloxy)benzene-1,4-dialdehyde (100 mg, 0.3 mmol) in 30 mL of acetic acid. The mixture was stirred at reflux for one night. The solution was concentrated and the pure product was precipitated by addition of water. The ligand L<sub>2</sub> was recovered by filtration, washed with cold ethanol and ether, and dried in vacuum. Yield: 200 mg (93 %). HR-ESI-MS ( $m/z$ ): 715.3448 [ $L_1-H$ ]<sup>+</sup> (715.3431, theor.). <sup>1</sup>H NMR (CD<sub>3</sub>CN, 300 MHz),  $\delta$  = 9.06-8.99 (m, 8H, H<sub>1,3</sub>), 8.01 (s, 2H, H<sub>4</sub>), 7.86 (q, 4H, *J* = 9 Hz, H<sub>2</sub>), 4.32 (t, 4H, *J* = 8.1 Hz, OCH<sub>2</sub>), 1.44 (m, 4H, CH<sub>2alkyl</sub>), 1.25-1.11 (m, 12H, CH<sub>2alkyl</sub>), 0.66 (t, 6H, *J* = 10.6 Hz, CH<sub>3alkyl</sub>). Anal. Calcd for C<sub>44</sub>H<sub>42</sub>N<sub>8</sub> : C, 73.93; H 5.92; N, 15.67. Found: C, 74.23; H 6.11; N, 15.88.

**Synthesis of (CD<sub>1</sub>.2PF<sub>6</sub>).** L<sub>1</sub> (100 mg, 0.14 mmol) and Ir<sub>2</sub>(dfppy)<sub>4</sub>μ-Cl<sub>2</sub> (170 mg, 0.14 mmol) were dispersed in a mixture of CHCl<sub>3</sub>/DMF/MeOH (v/v/v = 30/30/20 mL) and stirred at reflux overnight under nitrogen. NH<sub>4</sub>PF<sub>6</sub> was added to the resulting clear solution and the solvent was partially evaporated. EtOH (20 mL) was added to precipitate the complex which was filtered off, washed with ethanol and dried. Yield: 244 mg, (94 %). HR-ESI-MS ( $m/z$ ): 930.7168 [ $M$ ]<sup>2+</sup> (930.7152, theor.). Anal. Calcd for C<sub>90</sub>H<sub>61</sub>F<sub>20</sub>Ir<sub>2</sub>N<sub>13</sub>P<sub>2</sub> : C, 50.26; H 2.86; N, 8.47. Found: C, 50.33; H, 3.01; N, 8.65.

**Synthesis of (CD<sub>2</sub>.2PF<sub>6</sub>).** L<sub>2</sub> (30 mg, 0.042 mmol) and Ir<sub>2</sub>(dfppy)<sub>4</sub>μ-Cl<sub>2</sub> (52 mg, 0.042 mmol) were dispersed in a mixture of ethanol/dichloromethane (v/v = 15/15 mL) and stirred at reflux overnight under nitrogen. NH<sub>4</sub>PF<sub>6</sub> was added to the resulting clear solution and the solution was concentrated to precipitate the complex which was filtered off, washed with ethanol and dried. The complex was isolated pure as a yellow solid. Yield: 53mg, (59 %). HR-ESI-MS ( $m/z$ ): 930.2247 [ $M$ ]<sup>2+</sup> (930.2281, theor.). <sup>1</sup>H NMR (CD<sub>3</sub>CN)  $\delta$  = 9.29 (d, 2H, *J* = 7.1 Hz, H<sub>5</sub>), 9.04 (d, 2H, *J* = 8.6 Hz, H<sub>5</sub>'), 8.39-8.34 (m, 9H, H<sub>1,3</sub>), 7.98 (q, 4H, *J* = 5.2 Hz, H<sub>2</sub>), 7.89 (t, 4H, *J* = 7.5 Hz, H<sub>8</sub>), 7.62 (s, 2H, H<sub>4</sub>), 7.54 (m, 4H, H<sub>6</sub>), 6.96 (t, 4H, *J* = 6.5 Hz, H<sub>7</sub>), 6.78 (td, 4H, <sup>3</sup>*J* = 7.3 Hz, <sup>2</sup>*J* = 2.3 Hz, H<sub>9</sub>), 5.85 (dd, 4H, <sup>3</sup>*J* = 8.6 Hz, <sup>2</sup>*J* = 1.9 Hz, H<sub>10</sub>), 4.50 (m, 4H, OCH<sub>2</sub>), 2.30 (m, 4H, CH<sub>2alkyl</sub>), 1.23-1.66 (m, 12H, CH<sub>2alkyl</sub>), 0.85 (t, 6H, *J* = 7.1 Hz, CH<sub>3alkyl</sub>). <sup>13</sup>C NMR (CD<sub>3</sub>Cl)  $\delta$  = 170.1, 163.5, 160.5, 159.1, 155.5, 150.4, 149.9, 149.4, 139.2, 132.4, 127.9, 128.2, 123.5, 123.3, 113.5, 98.5, 98.2, 98.1, 69.7, 56.6, 31.0, 28.4, 25.3, 22.1, 17.4, 13.0. Anal. Calcd for C<sub>88</sub>H<sub>66</sub>F<sub>20</sub>Ir<sub>2</sub>N<sub>12</sub>O<sub>2</sub>P<sub>2</sub> : C, 49.16; H 3.09; N, 7.82. Found: C, 49.40; H, 3.47; N, 8.11.

**Synthesis of soft salt CD<sub>1</sub>.2A.** A mixture of CD<sub>1</sub>.2PF<sub>6</sub> (100 mg, 0.0459 mmol) and NBu<sub>4</sub>.A (86.6 mg, 0.0919 mmol) was stirred at room temperature for one hour in a mixture of water/CHCl<sub>3</sub> (v/v = 5/5 mL). The mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub> and washed with water several times. Organic phases were combined, dried over magnesium sulfate and the solvent was removed under reduced pressure. Yellow solid was used without any further purification. Anal. Calcd for C<sub>138</sub>H<sub>85</sub>F<sub>16</sub>Ir<sub>4</sub>N<sub>21</sub>S<sub>4</sub> : C, 51.18; H 2.65; N, 9.08; S, 3.96. Found: C, 52.06; H 2.93; N, 9.17; S, 4.18.

**Synthesis of soft salt CD<sub>2</sub>.2A.** A mixture of CD<sub>2</sub>.2PF<sub>6</sub> (100 mg, 0.0465 mmol) and NBu<sub>4</sub>.A (86.6 mg, 0.093 mmol) was stirred at room temperature for one hour in a mixture of water/CHCl<sub>3</sub> (v/v = 5/5 mL). The mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub> and washed with water several times. The organic phases were combined, dried over magnesium sulfate and the solvent removed under reduced pressure. Yellow solid was used without any further purification. Anal. Calcd for C<sub>136</sub>H<sub>90</sub>F<sub>16</sub>Ir<sub>4</sub>N<sub>20</sub>O<sub>2</sub>S<sub>4</sub>: C, 50.46; H 2.80; N, 8.65; S, 3.96. Found: C, 51.85; H 3.15; N, 8.96; S, 4.01.

### A-2-Device Fabrication and Measurements:

Prior to device fabrication, indium/tin oxide (ITO) glass substrates with sheet resistivity of 10-12 Ω/cm<sup>2</sup> were successively cleaned by sonication in acetone, ethanol and isopropanol for 15 min., and finally exposed to UV-ozone for 20 min. The poly(3,4-ethylenedioxythiophene)/poly(styrenesulfonate) (PEDOT:PSS) layer was spin-coated under ambient air onto the ITO substrates at a rate of 3000 rpm for 90 s (40 nm) then baked in air at 120°C for one hour to remove residual solvent. A filtered solution of poly(vinylcarbazole) (PVK, average M<sub>n</sub> = 25000-50000, 20 mg/mL in 1,2-dichlorobenzene) was then spin-coated at a rate of 3000 rpm for 40 s (20 nm). For device studies, each soft salt (CD<sub>1</sub>.2A. and CD<sub>2</sub>.2A.) was dissolved in 1,2-dichlorobenzene at a concentration of 30 mg/mL and the solutions were stirred for one hour before being filtered through a 0.45 μm poly(tetrafluorethylene) filter. To obtain a layer with a thickness of 65-70 nm, 60 μL of each solution was then deposited at 1500 rpm during 60s on the top of the PVK layer (20 nm). The assembly was transferred into a deposition chamber where the calcium cathode (300 nm) was deposited by thermal evaporation under secondary vacuum, followed by the deposition of aluminum (60 nm). The Ca (300 nm) / Al (60 nm) bilayer cathode of the device was evaporated through a shadow mask.

Current density–voltage–luminescence (*J*–*V*–*L*) characteristics of OLEDs were measured with a Keithley 4200 Semiconductor analyser coupled with a Hamamatsu Light sensor calibrated with a Minolta CS-100 luminancemeter. The EL spectra were collected with an Ocean Optics HR2000 Spectrometer. Chromatic Coordinates were calculated from the EL spectra and reported following the CIE-1964 chromaticity diagram. Devices are stored and characterized in nitrogen filled gloveboxes (O<sub>2</sub> and H<sub>2</sub>O < 0.1 ppm) without encapsulation.

## B- Physical data

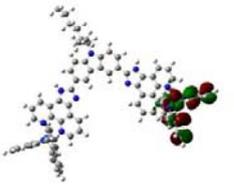
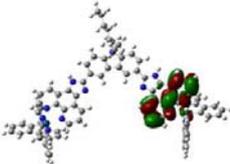
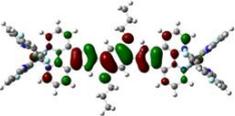
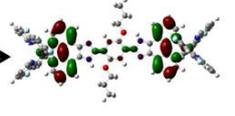
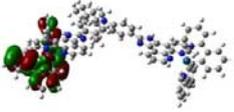
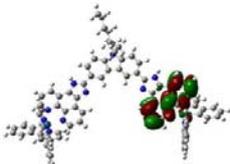
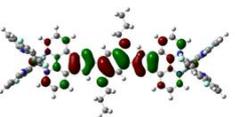
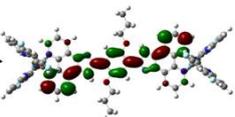
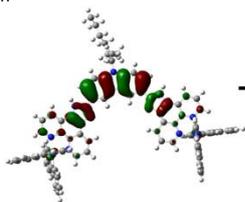
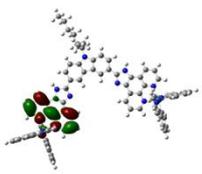
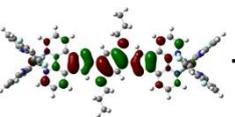
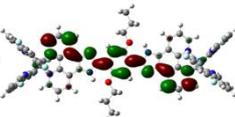
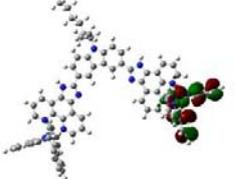
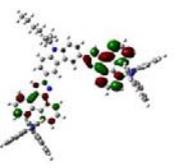
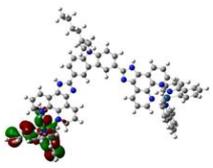
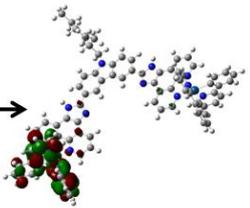
**Table 1:** Spectroscopic data of the samples

samples	$\lambda_{\text{abs}}$ [nm]	$\epsilon/\text{dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$
CD <sub>1</sub> .2PF <sub>6</sub>	459	7450
CD <sub>1</sub> .2PF <sub>6</sub>	431	10000
CD <sub>1</sub> .2PF <sub>6</sub>	384	32300
CD <sub>1</sub> .2PF <sub>6</sub>	360	51400
CD <sub>1</sub> .2PF <sub>6</sub>	319	72400
CD <sub>1</sub> .2PF <sub>6</sub>	295	91200
CD <sub>1</sub> .2PF <sub>6</sub>	267	93140
CD <sub>1</sub> .2PF <sub>6</sub>	250	93100
CD <sub>1</sub> .2A	459	7353
CD <sub>1</sub> .2A	432	1000
CD <sub>1</sub> .2A	384	34270
CD <sub>1</sub> .2A	361	57712
CD <sub>1</sub> .2A	295	124900
CD <sub>1</sub> .2A	249	170860
CD <sub>2</sub> .2PF <sub>6</sub>	451	10970
CD <sub>2</sub> .2PF <sub>6</sub>	420	41520
CD <sub>2</sub> .2PF <sub>6</sub>	394	58880
CD <sub>2</sub> .2PF <sub>6</sub>	343	43480
CD <sub>2</sub> .2PF <sub>6</sub>	291	85845
CD <sub>2</sub> .2PF <sub>6</sub>	264	96200
CD <sub>2</sub> .2PF <sub>6</sub>	247	112370
CD <sub>2</sub> .2A	453	10285
CD <sub>2</sub> .2A	390	42791
CD <sub>2</sub> .2A	390	42791
CD <sub>2</sub> .2A	343	43384
CD <sub>2</sub> .2A	289	107436
CD <sub>2</sub> .2A	250	169538
NBu <sub>4</sub> A	462	291
NBu <sub>4</sub> A	430	1242
NBu <sub>4</sub> A	385	3711
NBu <sub>4</sub> A	334	6880
NBu <sub>4</sub> A	251	40100

**Table 2:** Calculations of the main optical transitions of CD<sub>1</sub> and CD<sub>2</sub>

$\lambda$ (nm)	$f$	Transition (contribution)	assignment
<b>CD<sub>1</sub></b>			
452	0.135	HOMO-2→LUMO (45%)	L'LCT/MLCT
413	0.069	HOMO-4→LUMO (57%)	L'LCT/MLCT
		HOMO-3→LUMO+1 (31%)	L'LCT
403	0.623	HOMO-2→LUMO+2 (85%)	L'LCT/MLCT
395	0.060	HOMO-1→LUMO+5 (76%)	ILCT
<b>CD<sub>2</sub></b>			
428	0.790	HOMO→LUMO (64%)	ILCT
385	0.981	HOMO→LUMO+2 (82%)	ILCT/MLCT
345	0.243	HOMO→LUMO+4 (52%)	ILCT/MLCT

**Table 3:** HOMO-LUMO transitions and isocontour plots of the frontier orbitals of complexes  $CD_1$  and  $CD_2$ .

$CD_1$		$CD_2$	
<b>HOMO-2</b>	<b>LUMO</b>	<b>HOMO</b>	<b>LUMO</b>
			
<b>HOMO-4</b>	<b>LUMO#</b>	<b>HOMO</b>	<b>LUMO+2</b>
			
<b>HOMO-3</b>	<b>LUMO+1#</b>	<b>HOMO</b>	<b>LUMO+4</b>
			
<b>HOMO-2</b>	<b>LUMO+2#</b>		
			
<b>HOMO-1</b>	<b>LUMO+5</b>		
			

**Table 4:** Photoluminescence data

samples	$\lambda_{em}^a$ [nm]	$\Phi_F^b$	solid-state $\lambda_{em}$ [nm] <sup>c</sup>
<b>CD<sub>1</sub>.2PF<sub>6</sub></b>	547	0.091	nd
<b>CD<sub>1</sub>.2A</b>	476, 503	0.063	594
<b>CD<sub>2</sub>.2PF<sub>6</sub></b>	510	0.150	nd
<b>CD<sub>2</sub>.2A</b>	482,446	0.149	557
<b>NBu<sub>4</sub>A</b>	466	0.57	560

<sup>a</sup> in CH<sub>2</sub>Cl<sub>2</sub> (298K),  $\lambda_{exc}$  350 nm; <sup>b</sup> quantum yields (%) reference: Ru(bpy)<sub>3</sub>Cl<sub>2</sub>; <sup>c</sup>  $\lambda_{exc}$  350 nm, nd= not determined

**Table 5** Redox potentials and energy levels of frontier orbitals.

samples	$E_{red}^{\circ}(2)$ [V] <sup>a</sup>	$E_{red}^{\circ}(1)$ [V] <sup>a</sup>	$E_{ox}(1)$ [V] <sup>a</sup>	$E_{ox}(2)$ [V] <sup>a</sup>	Energy Levels (eV) HOMO/LUMO
<b>CD<sub>1</sub>.(PF<sub>6</sub>)<sub>2</sub></b>	-	-2.44 <sup>irr</sup>	1.25 <sup>irr</sup>	-	-5.5/-2.4
<b>CD<sub>2</sub>.(PF<sub>6</sub>)<sub>2</sub></b>	-2.55 <sup>irr</sup>	-2.11 <sup>irr</sup> , -2.02 <sup>irr</sup>	1.14 <sup>irr</sup>	1.41 <sup>irr</sup>	-5.4/-2.5
<b>NBu<sub>4</sub>.A</b>	-	-1.98 <sup>irr</sup>	1.01 <sup>irr</sup>	-	-5.2/-2.7
<b>CD<sub>1</sub>.2A</b>	-2.41 <sup>irr</sup>	-2.10 <sup>irr</sup> , -1.97 <sup>irr</sup>	1.14 <sup>irr</sup>	1.42 <sup>irr</sup>	-5.4/-2.5
<b>CD<sub>2</sub>.2A</b>	-2.67 <sup>irr</sup>	-2.12 <sup>irr</sup> , -1.96 <sup>irr</sup>	1.13 <sup>irr</sup>	1.41 <sup>irr</sup>	-5.3/-2.5

<sup>a</sup> CV in acetonitrile on carbon electrode vs SCE, with TBA, ClO<sub>4</sub> (0.1 M) as supporting electrolyte. Scan rate: 50 mV/s.  $E_{red}^{\circ}$  is the reduction standard potential.

## C- Spectroscopic data

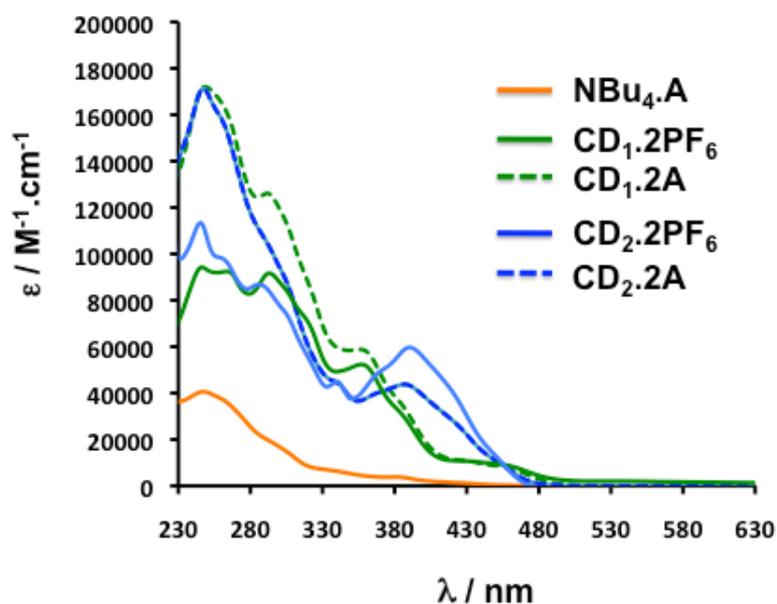


Figure SI 1. U.V.-visible absorption spectra of the different samples in  $\text{CH}_2\text{Cl}_2$ .

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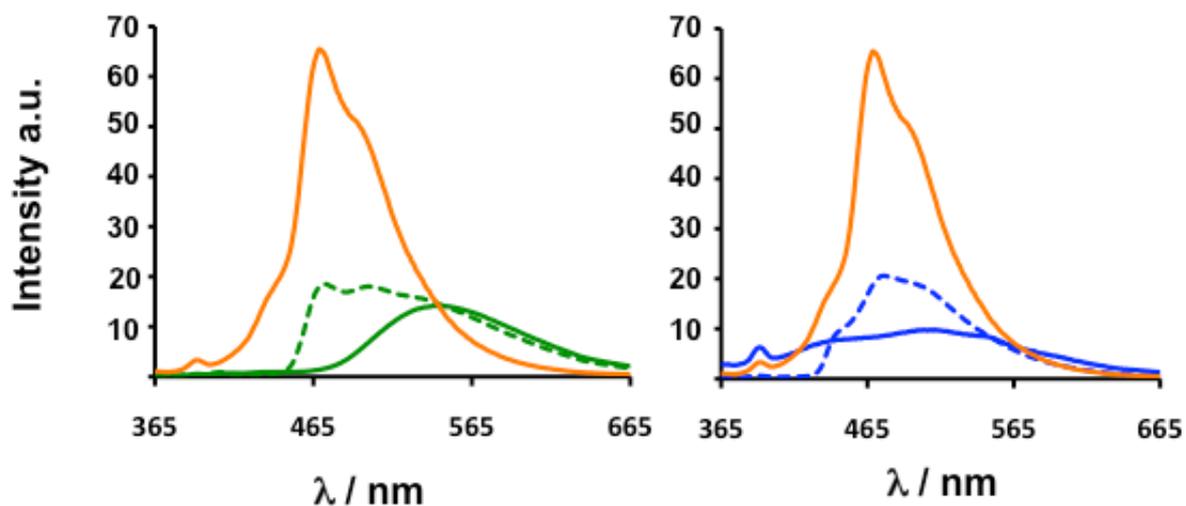


Figure SI2: Emission spectra (excitation at 350 nm) in degassed  $\text{CH}_2\text{Cl}_2$ ,  $\text{NBu}_4\cdot\text{A}$  (orange line),  $\text{CD}_{1.2}\text{PF}_6$  (green line),  $\text{CD}_{1.2}\text{A}$  (dotted green line),  $\text{CD}_{2.2}\text{PF}_6$  (blue line),  $\text{CD}_{2.2}\text{A}$  (dotted blue line).

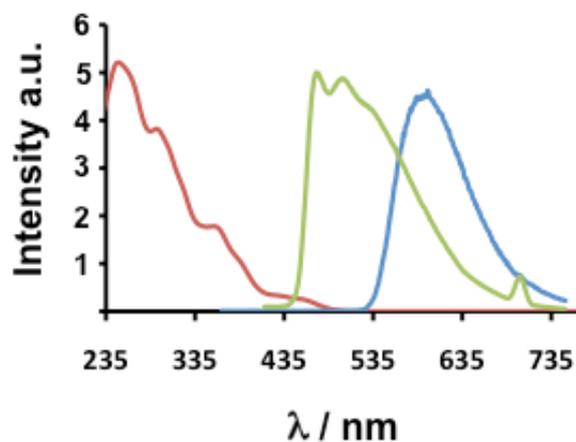


Figure SI3: Absorption spectra of CD<sub>1.2</sub>A (red line), photoluminescence spectra of CD<sub>1.2</sub>A (excitation at 350 nm) in degassed CH<sub>2</sub>Cl<sub>2</sub> (green line) and in solid state (blue line).

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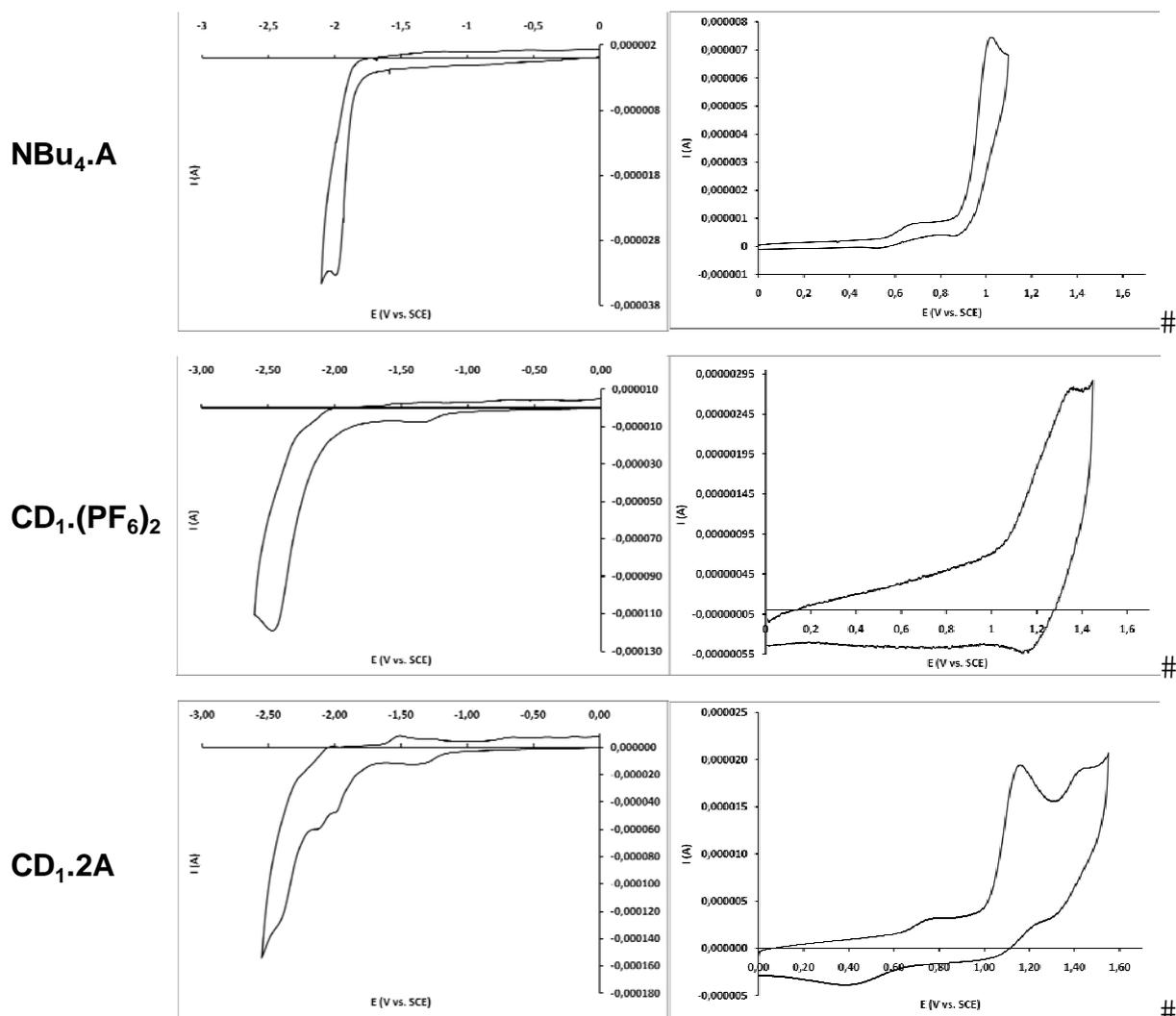


Figure SI 4. Cyclic voltammograms of NBu<sub>4</sub>.A (top), CD<sub>1.2</sub>PF<sub>6</sub> (middle), CD<sub>1.2</sub>A (down)

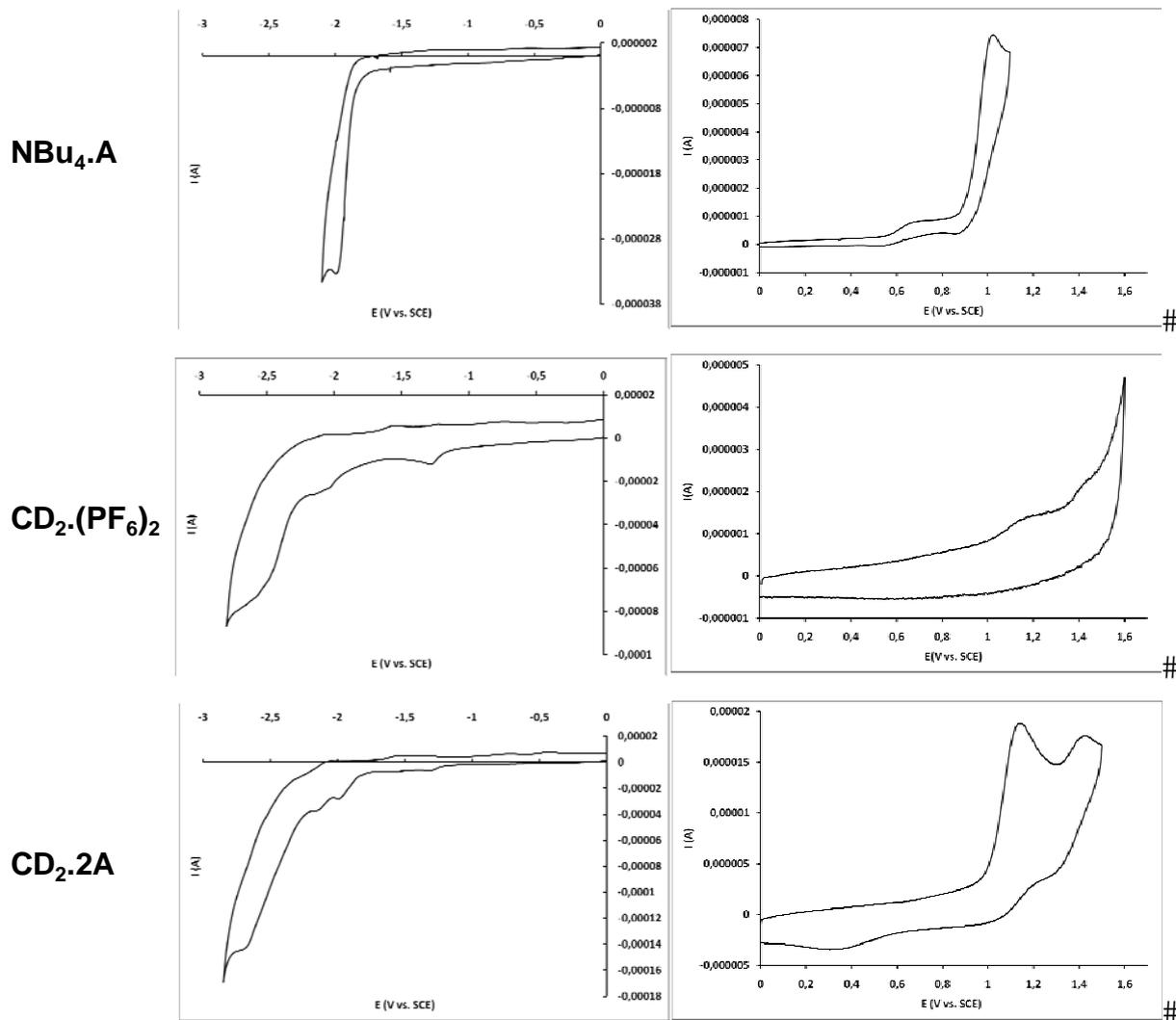


Figure SI 5. Cyclic voltammograms of  $\text{NBu}_4\cdot\text{A}$  (top),  $\text{CD}_2\cdot 2\text{PF}_6$  (middle),  $\text{CD}_2\cdot 2\text{A}$  (down)

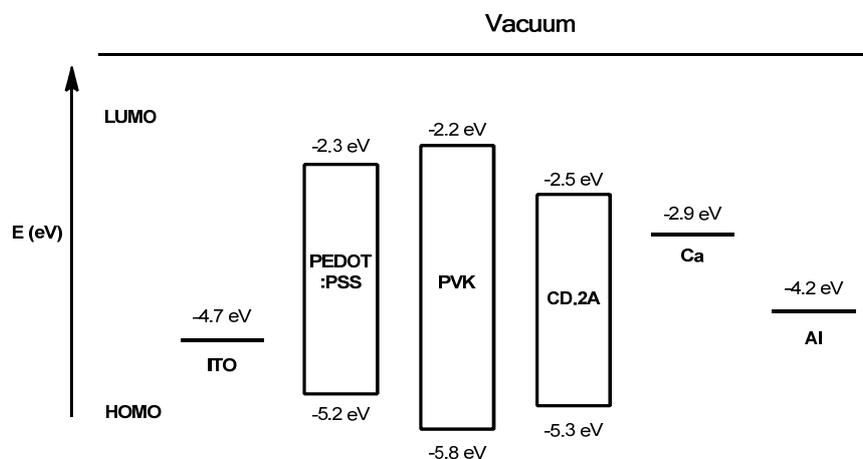
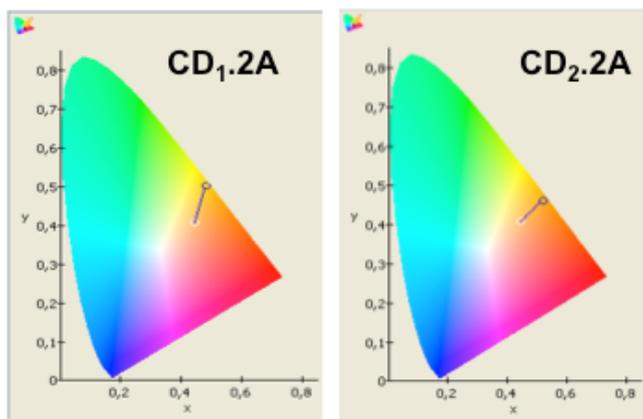


Figure SI 6: Energy band diagram of the materials and Fermi levels of the electrodes used in OLEDs. The highest and lowest occupied molecular orbitals (HOMO and LUMO) levels of CD.2A were calculated from their oxidation potentials.



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Figure SI 7: CIE diagrams of CD<sub>1.2A</sub> and CD<sub>2.2A</sub>

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