Blue electrofluorescence properties of furan-silole ladder pi-conjugated systems

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Table S1 Crystal data and structure refinement for 4

Identification code	201306101
Empirical formula	$C_{28}H_{18}O_2Si$
Formula weight	414.51
Temperature/K	291.15
Crystal system	monoclinic
Space group	C2/c
a/Å	18.2217(18)
b/Å	17.3887(12)
c/Å	7.6114(7)
α/°	90.00
β/°	119.638(13)
γ/°	90.00
Volume/Å^3	2096.1(3)
Z	4
ρ_{calc}mg/mm^3	1.313
m/mm^{-1}	0.135
F(000)	864.0
Crystal size/mm^3	0.22 × 0.2 × 0.2
2Θ range for data collection	5.86 to 52.74°
Index ranges	$-22 \le h \le 22$, $-12 \le k \le 21$, $-8 \le l \le 9$
Reflections collected	4465
Independent reflections	2143[R(int) = 0.0285]
Data/restraints/parameters	2143/0/141
Goodness-of-fit on F^2	1.015
Final R indexes [I>=2σ (I)]	R_1 = 0.0498, wR_2 = 0.1071
Final R indexes [all data]	R_1 = 0.0764, wR_2 = 0.1191
Largest diff. peak/hole / e Å^{-3}	0.25/-0.24

Table S2. Selected bond lengths [Å] and dihedral angles [°] for compounds **4**

	4
Si-C2	1.8692(19)
Si-C2a	1. 8692(19)
C1-C1a	1.445(4)
C3-C4	1.393(3)
C1-O1	1.365(2)
O1-C4	1.391(2)
C1-C2	1.346(3)
C1-C1a	1.445(4)
C5-C8	1.34
C5-02	1.36
O2-C6	1.39
C6-C7	1.39
C7-C8	1.44
Si-C_1-C_2-C_3	11.6°
Si-C_8-C_7-C_6	11.6

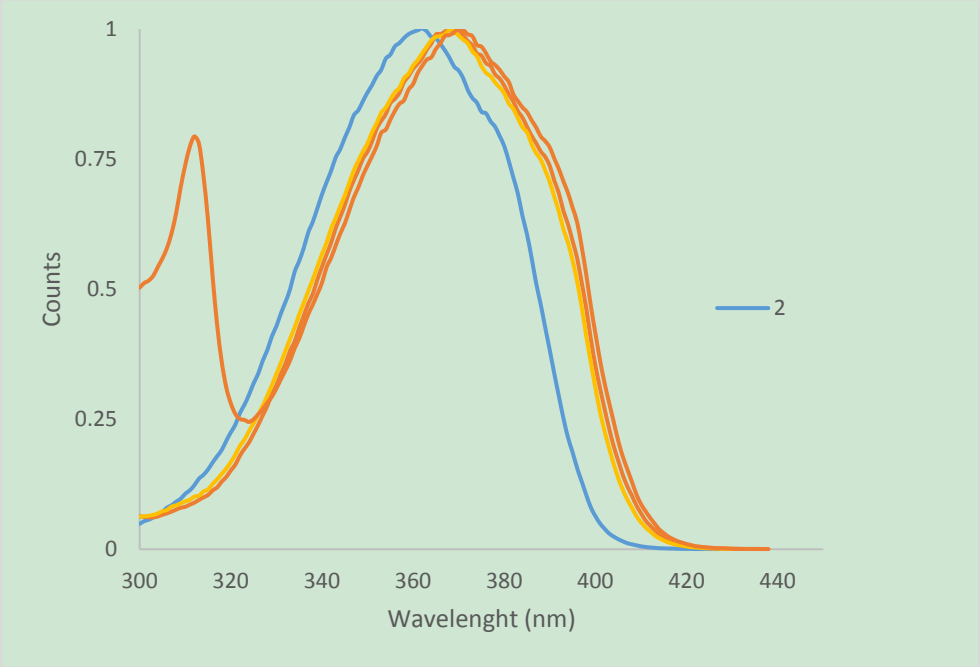


Figure S1 : Excitation scans recorded in DCM for **2**, **4-6**.

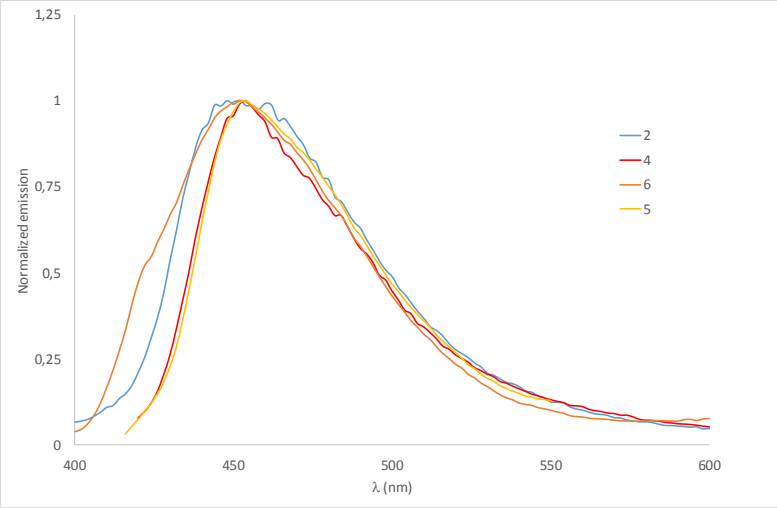


Figure S2: Solid-state luminescence spectra of **2**, **4-6**.

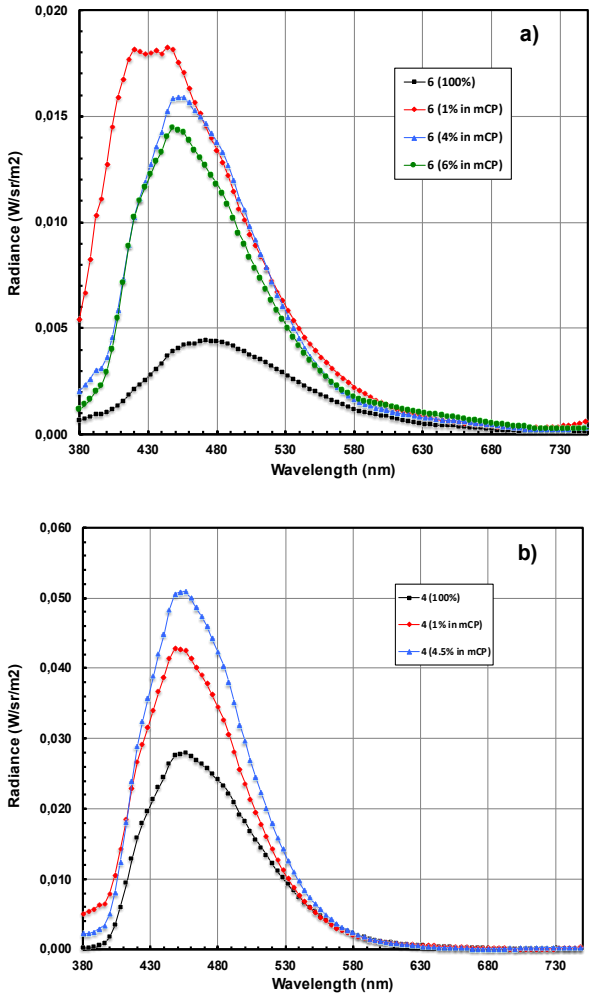


Figure S3. Electroluminescence spectra of the different devices recorded at 30 mA/cm2 for a) emitter **6** and b) emitter **4**.

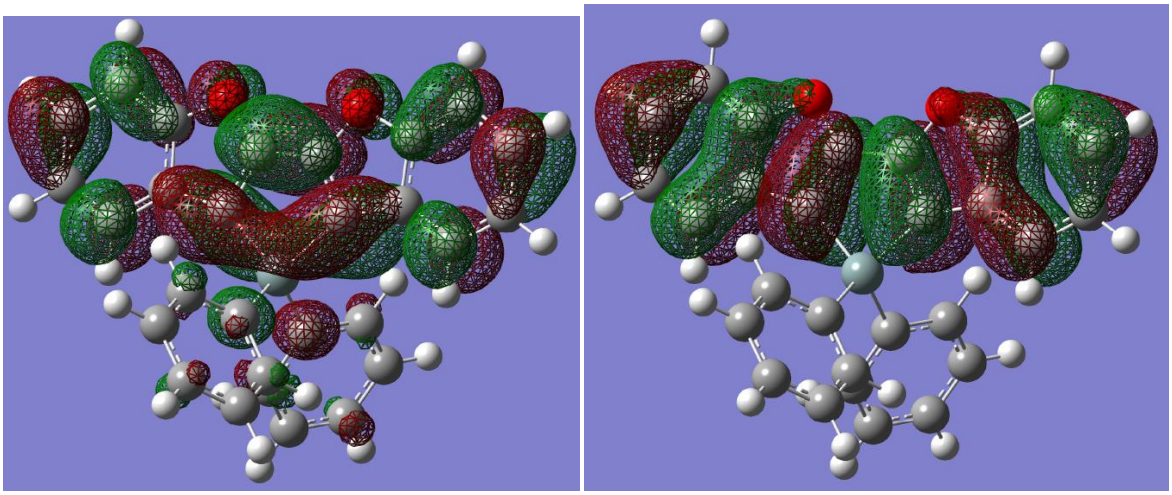
The molecular orbitals of **2** was calculated with Gaussian 09package at the b3lyp/6-311+g(d,p) level.[1]

C	2.75384816	0.13377966	0.00013303
C	2.82746777	-1.27818870	-0.00002647
C	4.01286102	-1.99242727	-0.00011288
C	5.18958358	-1.24482877	-0.00004422
C	5.15784081	0.15967771	0.00010387
C	3.95566483	0.85809905	0.00019144
C	1.34901101	0.45829521	0.00017611
C	0.72076531	-0.76154898	0.00000054
H	4.01854338	-3.07521176	-0.00022874
H	6.14440050	-1.75723106	-0.00010645
H	6.09302135	0.70799863	0.00015130
H	3.94810691	1.94201856	0.00029915
C	-4.01286024	-1.99242655	0.00010785
C	-2.82746053	-1.27819710	0.00000717
C	-5.18958231	-1.24482668	0.00010104
C	-2.75384364	0.13377096	-0.00012532
C	-5.15783746	0.15967808	-0.00001835
H	-6.14440002	-1.75722752	0.00019818
C	-3.95565693	0.85809436	-0.00014452
C	-1.34899933	0.45829478	-0.00026833
C	-0.72074306	-0.76153467	-0.00017788
H	-6.09301559	0.70800336	-0.00001742
H	-3.94809433	1.94201376	-0.00027147
O	1.56222814	-1.82907474	-0.00007790
O	-1.56225172	-1.82907774	0.00001993
Si	0.00000175	1.78762220	-0.00003783
H	-4.01854677	-3.07521110	0.00020281
C	-0.00028356	2.84845118	1.55236840
H	-0.00053252	2.22696449	2.45091900
H	0.88351722	3.49267602	1.58546732
H	-0.88401806	3.49278819	1.58505138
C	0.00026444	2.84874134	-1.55223468
H	-0.88350742	3.49301632	-1.58513355
H	0.88402746	3.49304293	-1.58484110
H	0.00042275	2.22744652	-2.45091781

The molecular orbitals of **4** was calculated with Gaussian 09package at the b3lyp/6-311+g(d,p) level.[1]

C	2.75256800	-1.01222200	-0.07675300
C	2.82715100	-2.42388800	-0.09082300
C	4.01248800	-3.13684900	-0.13318300
C	5.18750000	-2.38722900	-0.16485700
C	5.15418300	-0.98273100	-0.15367200
C	3.95222700	-0.28541100	-0.11008000
C	1.34837800	-0.69069800	-0.02466500
C	0.72090800	-1.91057800	-0.01684600
H	4.01945000	-4.21957300	-0.14206600
H	6.14246200	-2.89819900	-0.19973300
H	6.08829300	-0.43330000	-0.18105200
H	3.94162600	0.79820900	-0.10410500
C	-4.01236500	-3.13698800	0.13287400
C	-2.82704200	-2.42399600	0.09057600
C	-5.18739700	-2.38740300	0.16459800
C	-2.75250700	-1.01232600	0.07660700
C	-5.15412200	-0.98290400	0.15351900
H	-6.14234600	-2.89840300	0.19942900
C	-3.95218500	-0.28554800	0.10998200
C	-1.34832700	-0.69074700	0.02452600
C	-0.72080400	-1.91059400	0.01661100
H	-6.08824700	-0.43350100	0.18093700
H	-3.94161100	0.79807300	0.10408400
O	1.56222700	-2.97639400	-0.05514300
O	-1.56212400	-2.97645900	0.05485500
Si	0.00000400	0.63759800	0.00000400
C	-0.06499500	1.70235700	-1.55104500
C	0.71352800	2.86728200	-1.65629900
C	-0.85298400	1.33432600	-2.65362200
C	0.71099800	3.63174400	-2.82121700
H	1.32519500	3.18842900	-0.81893200
C	-0.85991400	2.09846000	-3.81967600
H	-1.46974800	0.44323600	-2.60152500
C	-0.07656800	3.24777700	-3.90584000
H	1.32026700	4.52697100	-2.88196900
H	-1.47765100	1.79727500	-4.65866400
H	-0.08131500	3.84314100	-4.81225600
C	0.06492500	1.70211900	1.55122100
C	-0.71335100	2.86720300	1.65650900
C	0.85260700	1.33372800	2.65389800
C	-0.71086500	3.63148400	2.82154600
H	-1.32479300	3.18861400	0.81907900

C	0.85948700	2.09767300	3.82007400
H	1.46916800	0.44249800	2.60178600
C	0.07639700	3.24716400	3.90626100
H	-1.31993800	4.52684400	2.88231900
H	1.47698600	1.79621100	4.65913700
H	0.08110900	3.84238800	4.81277100
H	-4.01930000	-4.21971400	0.14167500



LUMO HOMO

Figure S4. Calculated molecular orbitals of **4**

1.Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.