Electronic Supplementary Information (ESI)

3,4-Donor- and 2,5-acceptor-functionalized dipolar siloles: synthesis, structure, photoluminescence and electroluminescence

Gengwei Lin,[‡a] Long Chen,[‡a] Huiren Peng,[b] Shuming Chen,*[b] Zeyan Zhuang,[a] Yinghao Li,[a] Bohan Wang,[a] Zujin Zhao*[a] and Ben Zhong Tang*[ac]

[a] *State Key Laboratory of Luminescent Materials and Devices, South China University of Technology, Guangzhou 510640, China. Email: mszjzhao@scut.edu.cn.*

[b] *Department of Electrical and Electronic Engineering, South University of Science and Technology of China, Shenzhen, Guangdong 518055, China. Email: chen.sm@sustc.edu.cn.*

[c] *Department of Chemistry, Hong Kong Branch of Chinese National Engineering Research Center for Tissue Restoration and Reconstruction, The Hong Kong University of Science & Technology, Clear Water Bay, Kowloon, Hong Kong, China. Email: tangbenz@ust.hk.*

‡ Both authors contributed equally to this work.

Materials and instruments.

Tetrahydrofuran (THF) was distilled from sodium benzophenone ketyl under dry nitrogen immediately prior to use. Compound **1** was prepared according to the known procedures. All other chemicals and reagents were purchased from commercial sources and used as received without further purification. NMR spectra were obtained on a Bruker AV 500 or 600 spectrometer. High resolution mass spectra (HRMS) were recorded on a GCT premier CAB048 mass spectrometer operating in MALDI–TOF mode. Single crystal X-ray diffraction intensity data were collected on APEX2 CCD detector diffractometer using graphite monochromated MoKα radiation. Absorption correction was applied using the multi-scan method (SADABS). Structures were solved by direct methods

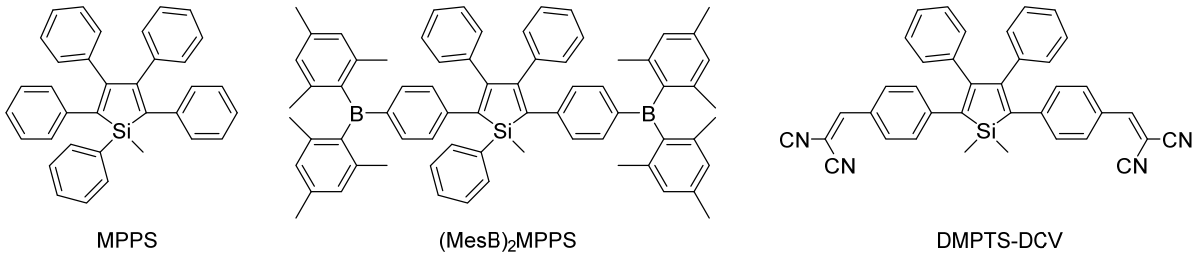
(SHELXS97) and refined by full-matrix least squares on F^2 (SHELXL97). UV–vis absorption spectra were measured on a SHIMADZU UV-2600 spectrophotometer. Fluorescence spectra were recorded on a Horiba Fluoromax-4 fluorescence spectrophotometer. Fluorescence quantum yields were measured using a Hamamatsu absolute PL quantum yield spectrometer C11347 Quantaurus_QY. Fluorescence lifetimes were determined with a Hamamatsu C11367-11 Quantaurus-Tau time-resolved spectrometer and the spectra were fitted with double exponential function. TGA analysis was carried out on a TA TGA Q5000 and DSC analysis was performed on a DSC Q1000 under dry nitrogen at a heating rate of 10 °C min^{-1}. The ground-state geometries were optimized using the density functional with B3LYP hybrid functional at the basis set level of 6–31G(d). All the calculations were performed using Gaussian 09 package. Cyclic voltamogramms were measured on a CHI 610E A14297 in a solution of tetra-*n*-butylammonium hexafluorophosphate (Bu_4NPF_6) (0.1 M) in dichloromethane at a scan rate of 100 mV s^{-1}.

Devices fabrication.

Multilayer OLEDs were fabricated by the vacuum-deposition method. Organic layers were deposited by high-vacuum (5×10^{-4} Pa) thermal evaporation onto a glass substrate pre-coated with an indium tin oxide (ITO) layer. All organic layers were deposited sequentially. Thermal deposition rates for the organic materials, LiF and Al were 0.5, 0.5 and 1 Å s^{-1}, respectively. The active area of each device was 12 mm^2. The electroluminescence spectra were measured on a Hitachi MPF-4 spectrofluorometer. The current density-voltage characteristics of the OLEDs were recorded on a Keithley 2400 Source Meter. The current density-voltage-luminance curves characterizations were carried out with a 3645

DC power supply combined with a 1980A spot photometer and they were recorded simultaneously. All measurements were done at room temperature under ambient conditions.

Additional data.



Scheme S1. Chemical structures of MPPS, $(MesB)_2MPPS$ and DMPTS-DCV.

Table S1 Optical properties of $(DPA)_2(CN)_2MPPS$, $(DPA)_2(MesB)_2MPPS$, $(MesB)_2MPPS$ and DMPTS-DCV.

Compound	λ_{em} (nm)		Φ_F (%)		α_{AIE} [a]	Ref.
	THF	Film	THF	Film		
$(DPA)_2(CN)_2MPPS$	459, 565	558	6.5	22.5	3.5	This paper
$(DPA)_2(MesB)_2MPPS$	454, 565	552	4.6	27.2	5.9	This paper
MPPS	491	491	0.09	85.0	944.4	1
$(MesB)_2MPPS$	516	524	1.35	58	43.0	2
DMPTS-DCV	553	581	1.4	8.5	6.1	3

[a] α_{AIE}: AIE effect reckoned through Φ_F (film)/Φ_F (THF).

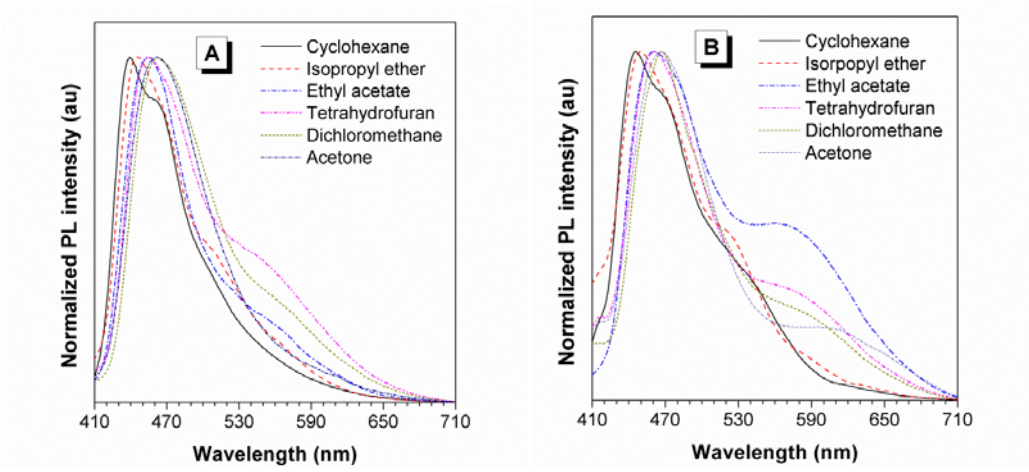


Fig. S1 PL spectra of (A) $(DPA)_2(MesB)_2MPPS$ and (B) $(DPA)_2(CN)_2MPPS$ in different solvents.

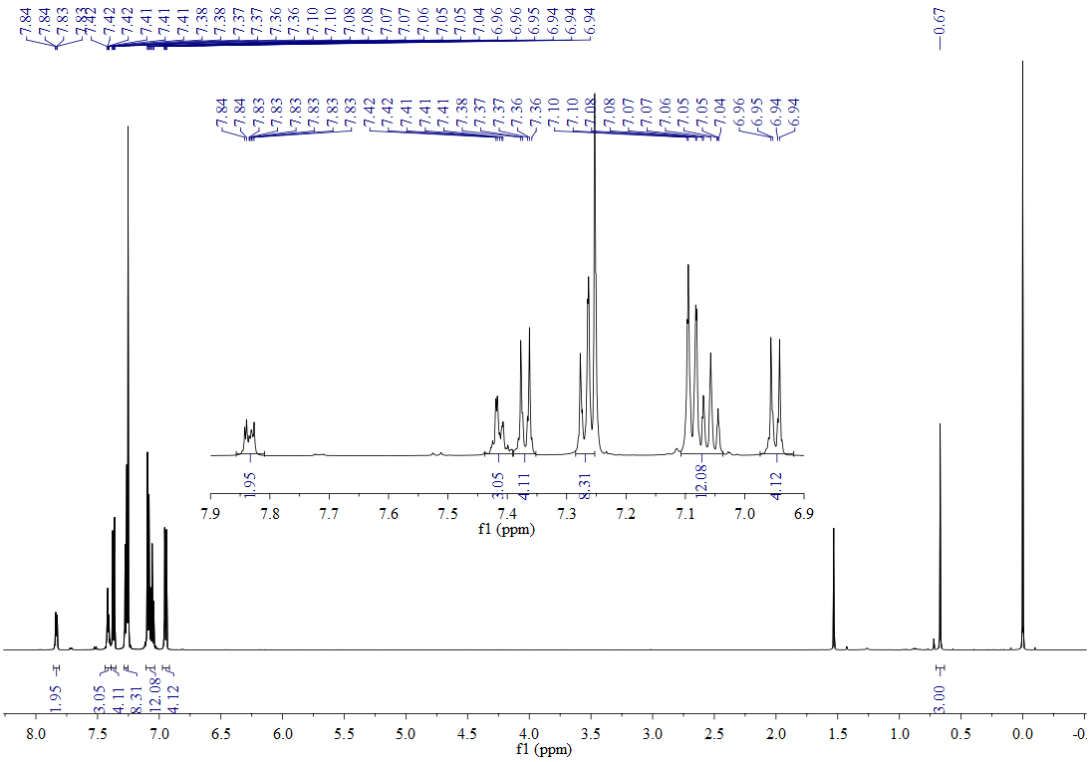


Fig. S2 ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

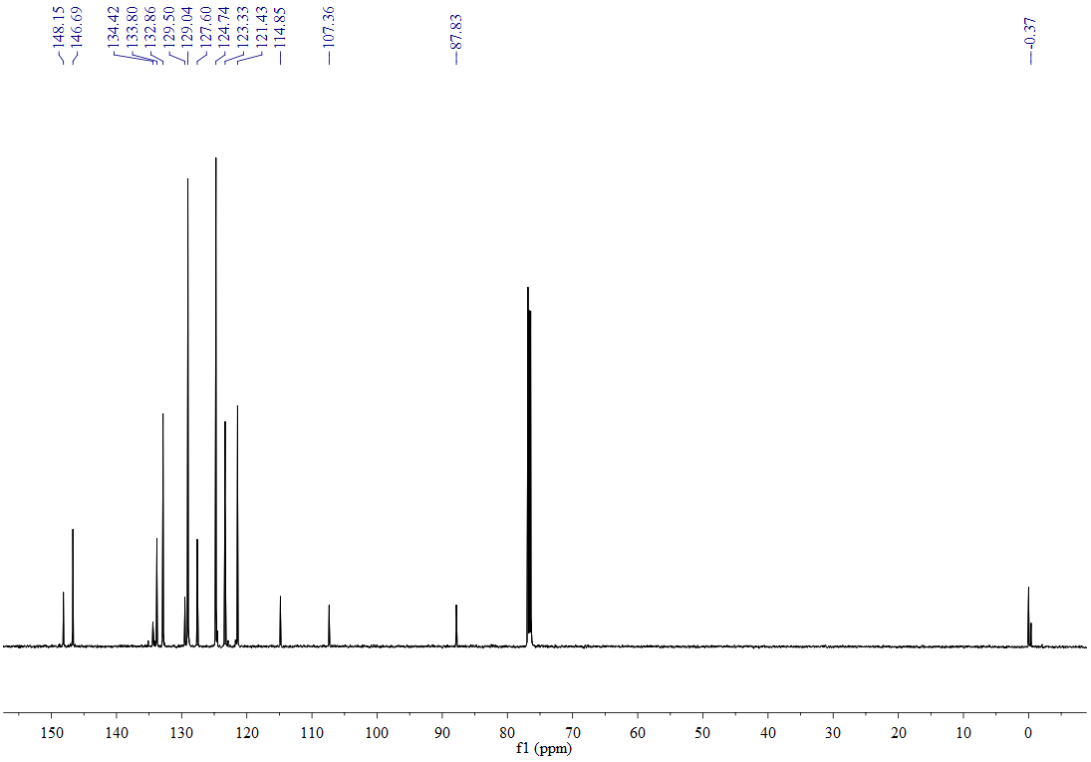


Fig. S3 ^{13}C NMR spectrum of compound **3** in $CDCl_3$.

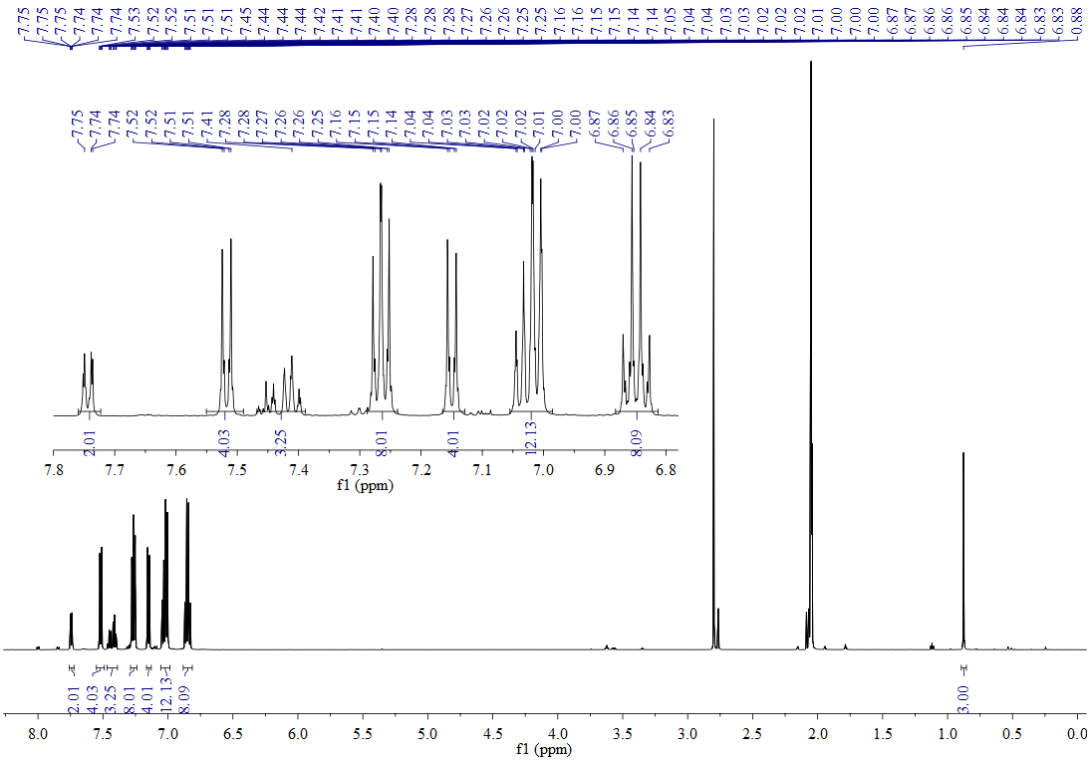


Fig. S4 ^{1}H NMR spectrum of $(DPA)_2(CN)_2MPPS$ in acetone-d_6.

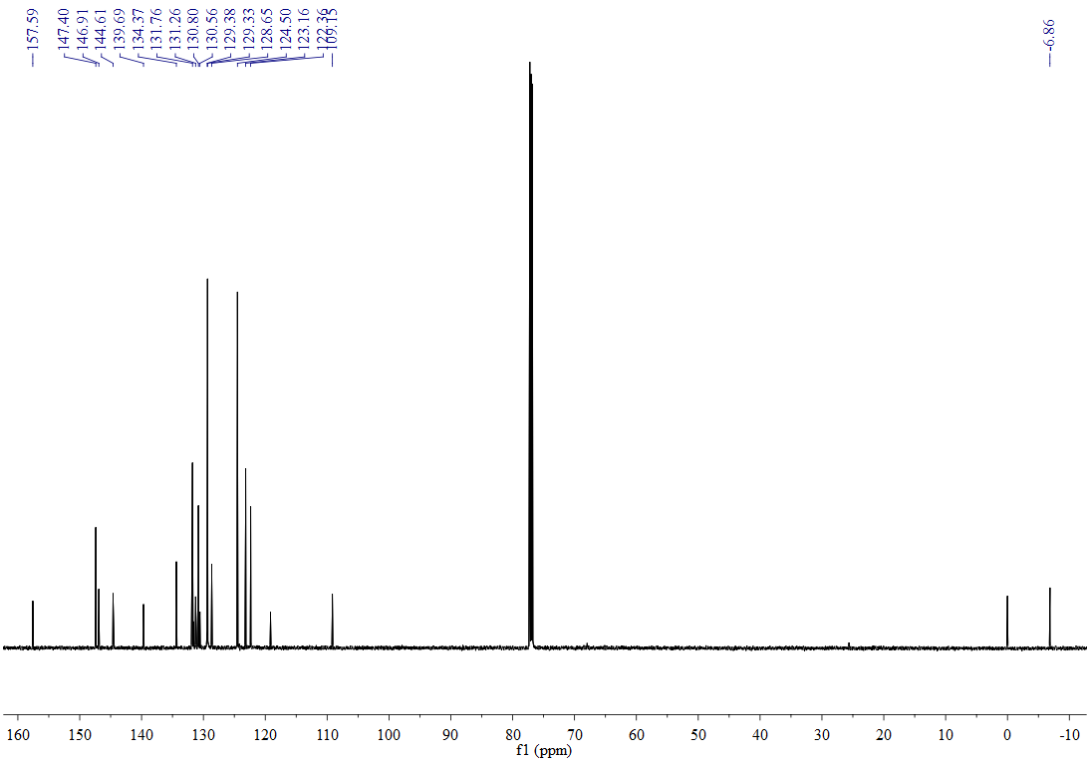


Fig. S5 ^{13}C NMR spectrum of $(DPA)_2(CN)_2MPPS$ in $CDCl_3$.

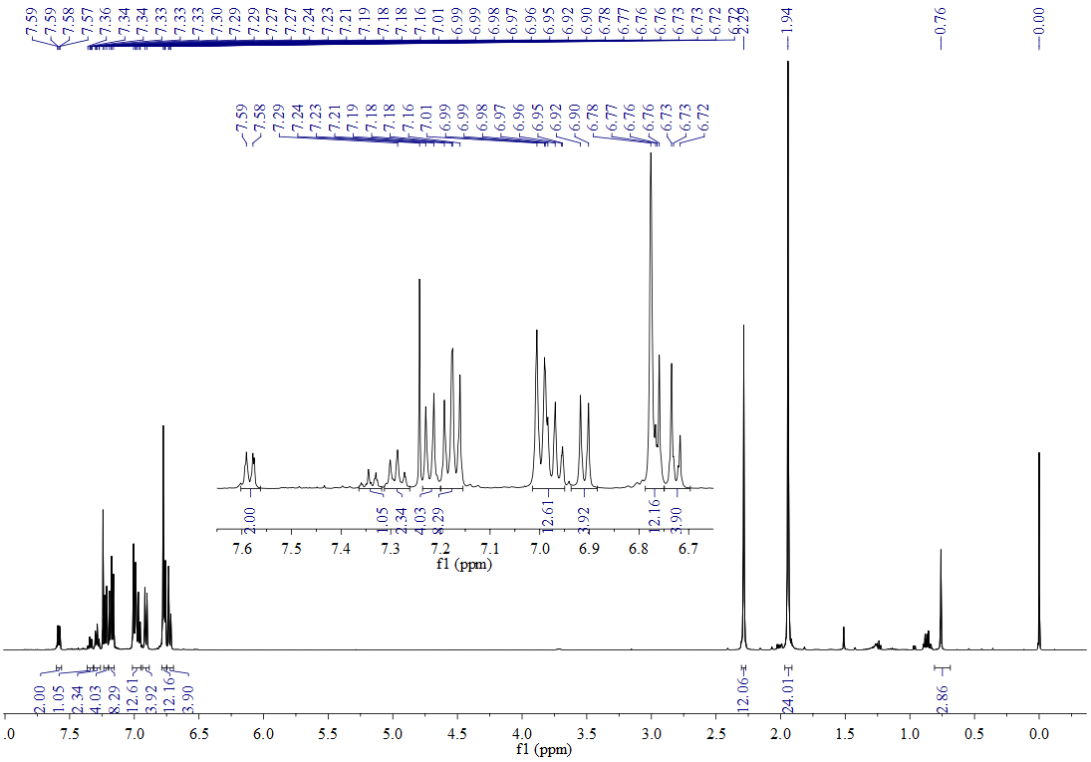


Fig. S6 ^{1}H NMR spectrum of $(DPA)_2(MesB)_2MPPS$ in $CDCl_3$.

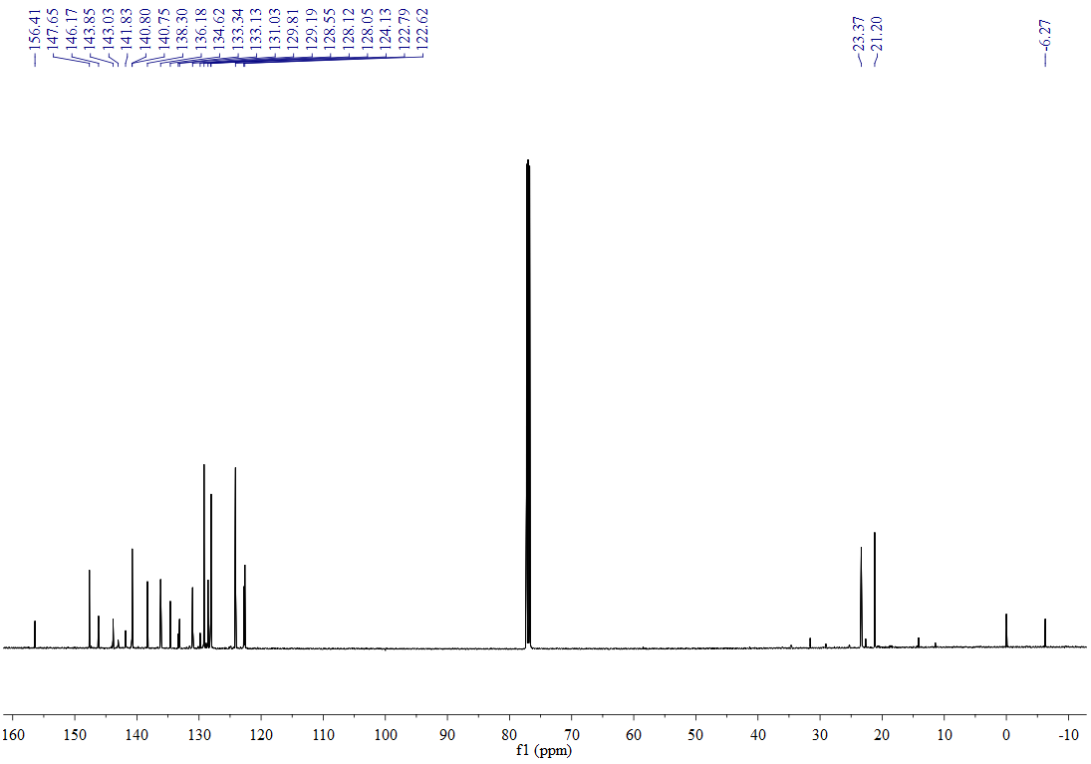


Fig. S7 ^{13}C NMR spectrum of $(DPA)_2(MesB)_2MPPS$ in $CDCl_3$.

References

1. Z. Zhao, S. Chen, J. W. Y. Lam, C. K. W. Jim, C. Y. K. Chan, Z. Wang, P. Lu, C. Deng, H. S. Kwok, Y. Ma and B. Z. Tang, *J. Phys. Chem. C*, 2010, **114***,* 7963.
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3. J. Mei, J. Wang, J. Z. Sun, H. Zhao, W. Yuan, C. Deng, S. Chen, H. H. Y. Sung, P. Lu, A. Qin, H. S. Kwok, Y. Ma, I. D. Williams and B. Z. Tang, *Chem. Sci.*, 2012, **3**, 549.