

# Supporting Information

for

## A Comparison between Triphenylmethyl and Triphenylsilyl Spirobifluorenyl Hosts: Synthesis, Photophysics and Performance in Phosphorescent Organic Light-Emitting Diodes

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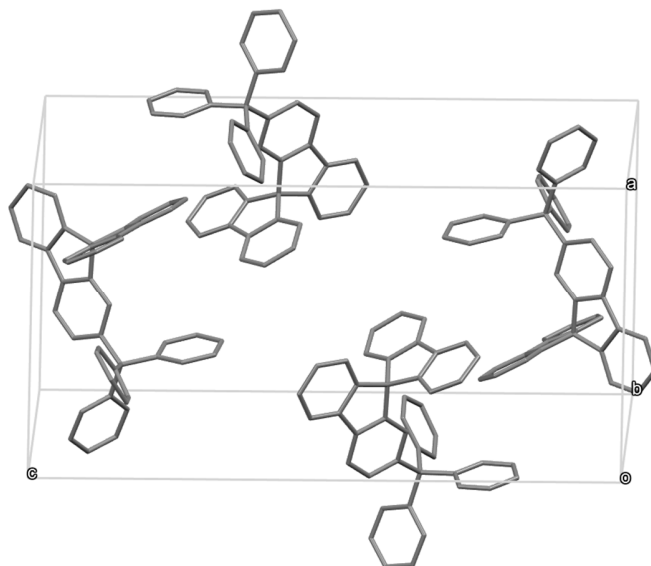
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Table S1: Crystallographic Data for **SB-C** and **SB-Si**.

Identification Code	SB-C	SB-Si
Empirical formula	C <sub>44</sub> H <sub>30</sub>	C <sub>43</sub> H <sub>30</sub> Si
Formula weight	558.68	574.76
Temperature/K	101(1)	102(2)
Crystal system	Monoclinic	monoclinic
Space group	P2 <sub>1</sub> /n	P2 <sub>1</sub> /n
a/Å	13.2736(3)	13.54470(12)
b/Å	9.03871(19)	9.29422(8)
c/Å	24.5142(6)	24.5334(2)
$\alpha$ /°	90	90
$\beta$ /°	91.929(2)	91.1600(8)
$\gamma$ /°	90	90
Volume/Å <sup>3</sup>	2939.45(11)	3087.81(5)
Z	4	4
$\rho_{\text{calc}}/\text{cm}^3$	1.262	1.236
$\mu/\text{mm}^1$	0.541	0.888
F(000)	1176.0	1208.0
Crystal size/mm <sup>3</sup>	0.164 × 0.11 × 0.039	0.576 × 0.201 × 0.1
Radiation	Cu K $\alpha$ ( $\lambda$ = 1.54184)	Cu K $\alpha$ ( $\lambda$ = 1.54184)
2 $\theta$ range for data collection/°	7.216 to 160.454	7.208 to 160.704
Index ranges	-16 ≤ h ≤ 16, -11 ≤ k ≤ 7, -31 ≤ l ≤ 30	-17 ≤ h ≤ 16, -8 ≤ k ≤ 11, -31 ≤ l ≤ 31
Reflections collected	23585	49890
Independent reflections	6180 [R <sub>int</sub> = 0.0386, R <sub>sigma</sub> = 0.0349]	6740 [R <sub>int</sub> = 0.0498, R <sub>sigma</sub> = 0.0289]
Data/restraints/parameters	6180/0/398	6740/0/398
Goodness-of-fit on F <sup>2</sup>	1.051	1.057
Final R indexes [I ≥ 2 $\sigma$ (I)]	R <sub>1</sub> = 0.0408, wR <sub>2</sub> = 0.1035	R <sub>1</sub> = 0.0390, wR <sub>2</sub> = 0.1011
Final R indexes [all data]	R <sub>1</sub> = 0.0489, wR <sub>2</sub> = 0.1078	R <sub>1</sub> = 0.0418, wR <sub>2</sub> = 0.1032
Largest diff. peak/hole/e Å <sup>-3</sup>	0.30/-0.21	0.45/-0.35
#CCDC	2221201	2216982

### SB-C Unit Cell



### SB-Si Unit Cell

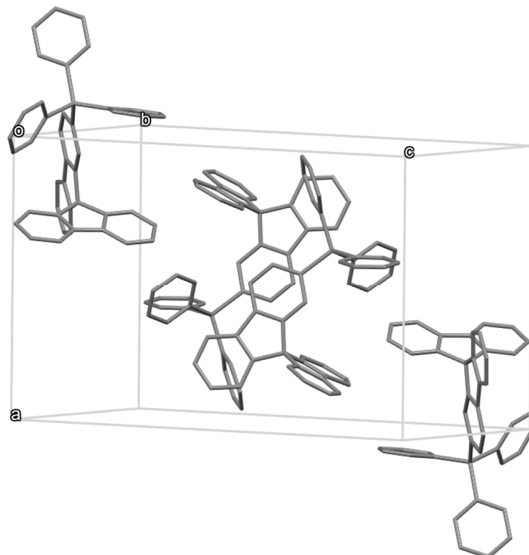


Figure S1. Packing of **SB-C** (top) and **SB-Si** (bottom) molecules in a unit cell.

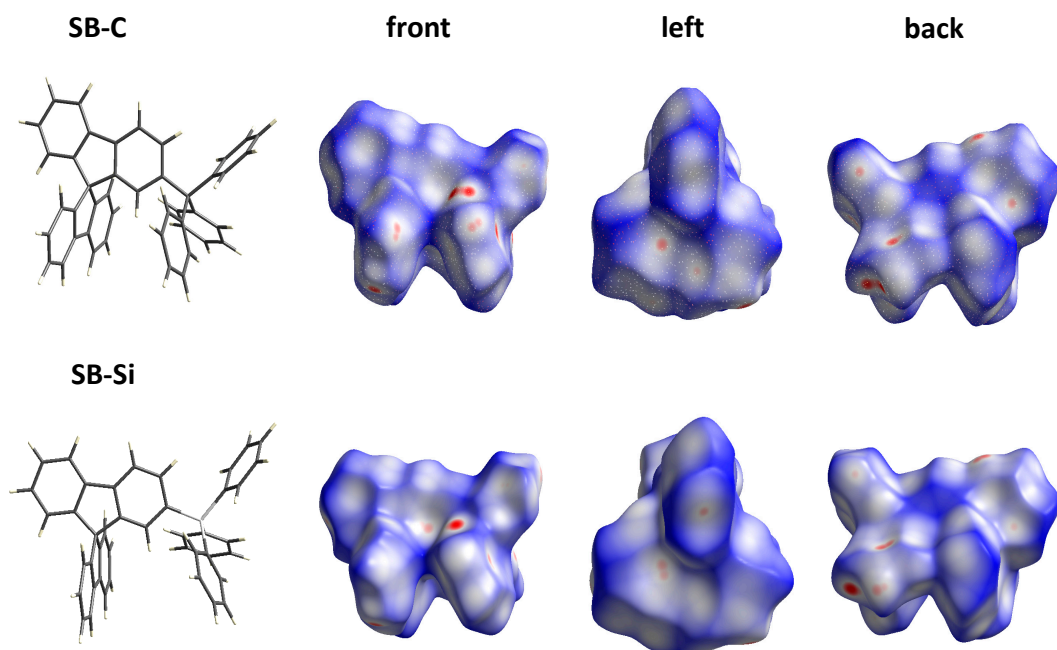


Figure S2. Calculated Hirshfeld surfaces of **SB-C** and **SB-Si**, which are shown in different viewing angles (front, left and back).

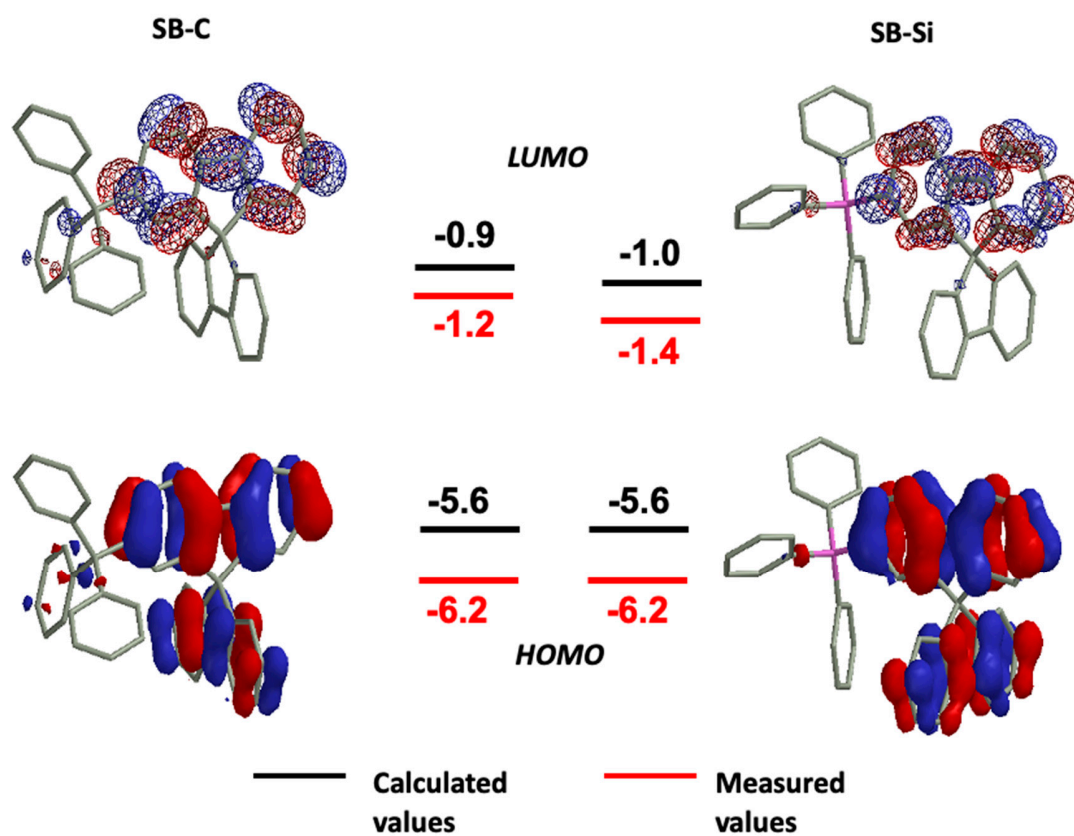


Figure S3. DFT calculated HOMO (solid) and LUMO (mesh) surface and levels of **SB-C** and **SB-Si**. Calculated values are compared to the measured values.

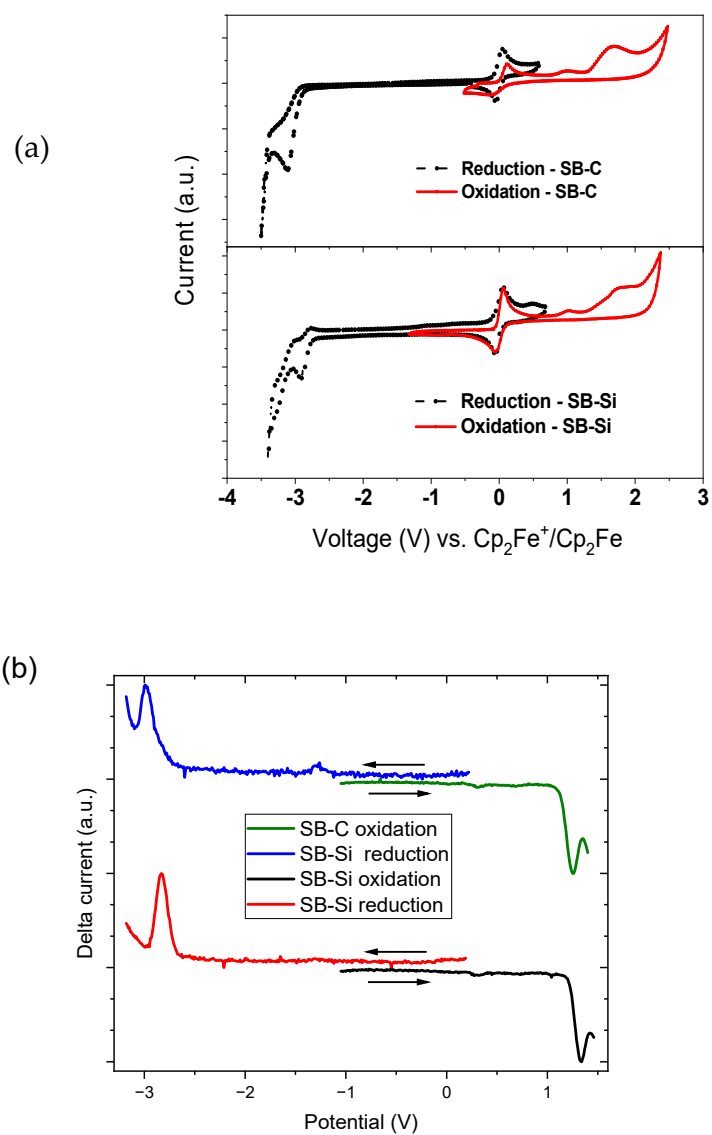


Figure S4. (a) Cyclic voltammetry and differential pulse voltammetry, (b), curves for **SB-Si** and **SB-C**.

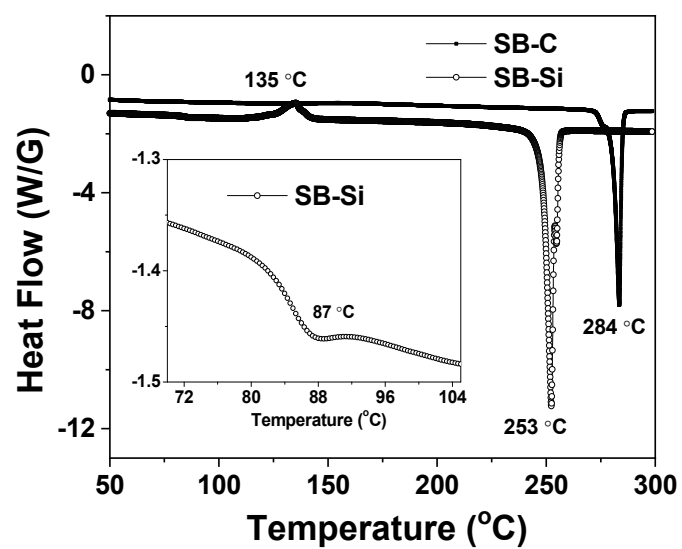


Figure S5. Differential scanning calorimetric (DSC) thermograms of **SB-Si** and **SB-C**.



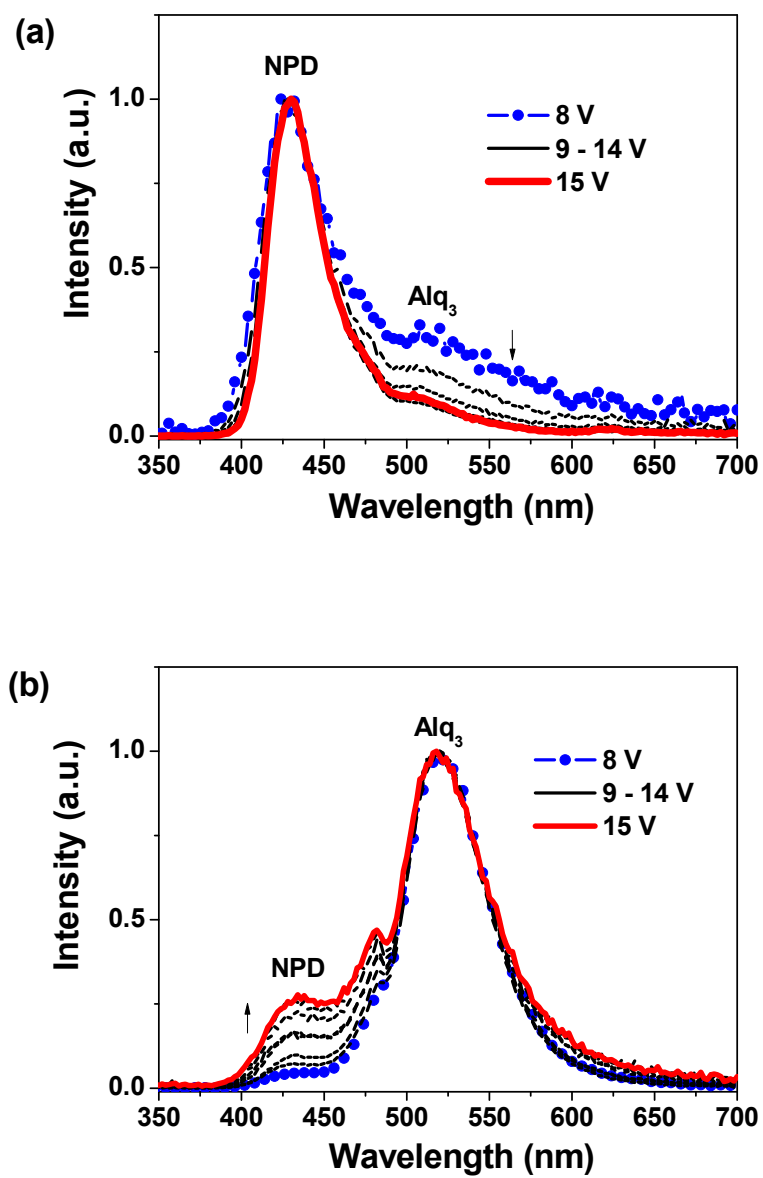


Figure S6. (a,b) Voltage dependence of EL spectra of the undoped devices.