Supporting information

Design strategy of exciton blocking materials using simulation and analysis of device properties

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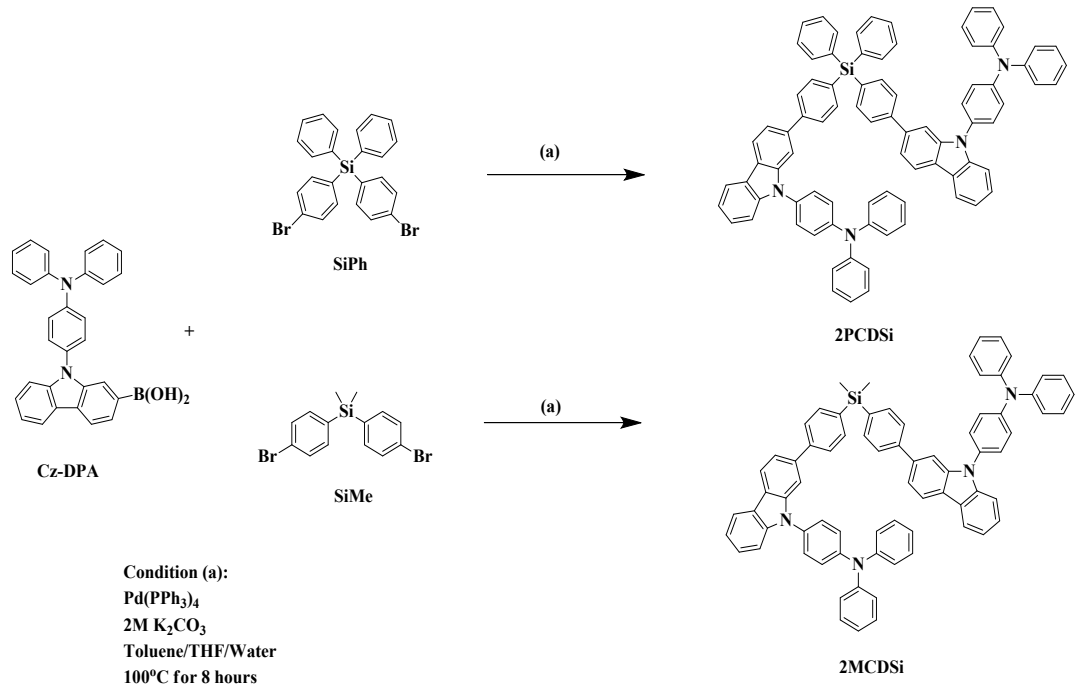
Synthetic Procedure



Scheme 1. The synthetic procedures of traget materials, **2PCDSi** and **2MCDSi**.

Synthesis of 2PCDSi

A mixture of bis(4-bromophenyl)diphenylsilane **SiPh** (2.0 g, 4.05 mmol), (9-(4-(diphenylamino)phenyl)-9H-carbazol-2-yl)boronic acid **Cz-DPA** (4.04 g, 8.90 mmol), tetrakis(triphenylphosphine)palladium(0) $Pd(PPh_3)_4$ (0.28 g, 0.24 mmol), potassium carbonate (13.82 g, 2M in 50 ml water), 20 ml of THF and 80 ml of toluene were added in to a two neck 250 ml round bottom flask equipped with condenser. Then, the mixture was refluxed for 8 hours under an inert condition. Reaction progress was monitored using TLC and after the reaction completion, reaction mixture was worked-up using chloroform (100 ml) and water (50 ml). The collected organic layer was dried over anhydrous sodium sulfate. After filtration through a celite pad, crude mixture was concentrated under vacuum condition using a rotary evaporator. After complete evaporation, crude mixture was dissolved well in chloroform and filtered through a silica pad. Finally, the target molecule of **2PCDSi** was obtained from recrystallization using minimum amount of chloroform and *n*-Hexane.

Yield: 67 %; Colourless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (d, *J*=8 Hz, 2H), 8.15 (d, *J*=8 Hz, 2H), 7.68-7.72 (m, 8H), 7.65 (d, *J*=8 Hz, 6H), 7.56 (d, *J*=8 Hz, 2H), 7.41-7.48 (m, 14H), 7.31 (t, *J*=8.5 Hz, 10H), 7.25 (d, *J*=8 Hz, 4H), 7.20-7.22 (m, 8H), 7.06 (t, *J*=7.5 Hz, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.3, 147.1, 143.0, 141.6, 141.5, 138.9, 136.8, 136.3, 134.1, 132.6, 130.9, 129.6, 129.4, 127.9, 127.8, 127.0, 125.9, 124.8, 123.6, 123.4, 122.8, 122.6, 120.5, 120.2, 119.8, 119.4, 109.8,

108.3; HRMS $[M+H]^+$ *m/z*: Anal. calcd. For $C_{84}H_{60}N_4Si$, 1152.4587; found, 1153.4664.

Synthesis of 2MCDSi

A mixture of bis(4-bromophenyl)dimethylsilane **SiMe** (2.0 g, 5.43 mmol), (9-(4-(diphenylamino)phenyl)-9H-carbazol-2-yl)boronic acid **Cz-DPA** (5.43 g, 11.96 mmol), Tetrakis(triphenylphosphine)palladium(0) $Pd(PPh_3)_4$ (0.50 g, 0.43 mmol), potassium carbonate (13.82 g, 2M in 50 ml water) and 100 ml of toluene were added in to a two neck 250 ml round bottom flask equipped with condenser. Then, the mixture was refluxed for 8 hours under an inert condition. Reaction progress was monitored using TLC and after the reaction completion, reaction mixture was worked-up using ethylacetate (80 ml) and water (50 ml) twice. The collected organic layer was dried over anhydrous sodium sulfate. After filtration through a celite pad, crude mixture was concentrated under vacuum condition using a rotary evaporator. After complete evaporation, crude mixture was dissolved well in minimum amount of ethylacetate and *n*-hexane was added slowly, stirred at room temperature for overnight, and then the collected precipitated was well washed with *n*- hexane. Again, the precipitate was dissolved in hot toluene and stirred at room temperature after adding little amount of *n*-hexane to obtain the target molecule of **2MCDSi**.

Yield: 74 %; Colourless solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J*=8 Hz, 2H), 8.13 (d, *J*=8 Hz, 2H), 7.74-7.81 (m, 4H), 7.61-7.63 (m, 8H), 7.38-7.53 (m, 16H), 7.25-7.32 (m, 10H), 7.19-7.23 (m, 4H), 7.04-7.07 (m, 4H), 0.62 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.6, 149.4, 145.1, 143.8, 141.4, 138.9, 136.9, 133.2, 131.8, 131.7, 130.2, 130.1, 129.6, 129.5, 128.1, 127.2, 127.1, 126.0, 125.7, 125.1, 124.7, 122.5, 122.1, 121.7, 112.1, 110.6, 2.2; HRMS (ESI) *m/z*: Anal. calcd. For $C_{74}H_{56}N_4Si$, 1028.4274; found, 1028.4277.

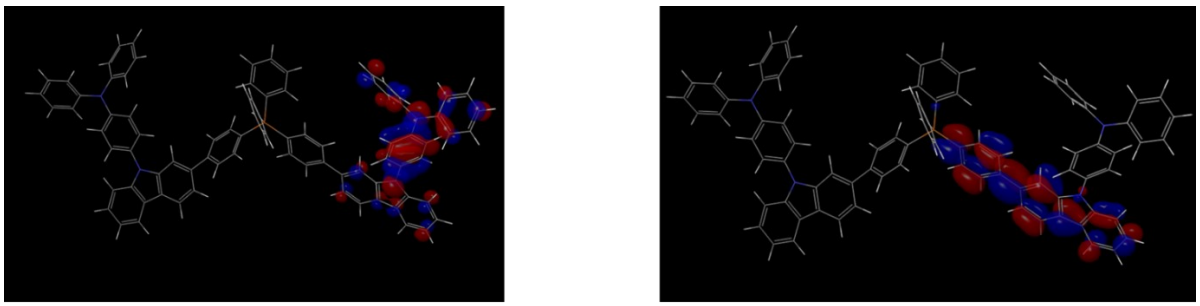


Figure S1. HOMO and LUMO distribution of 2PCDSi.

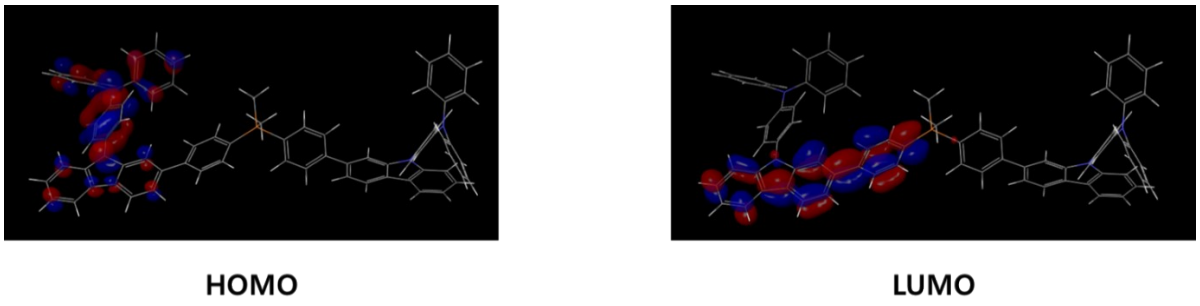


Figure S2. HOMO and LUMO distribution of 2MCDSi.

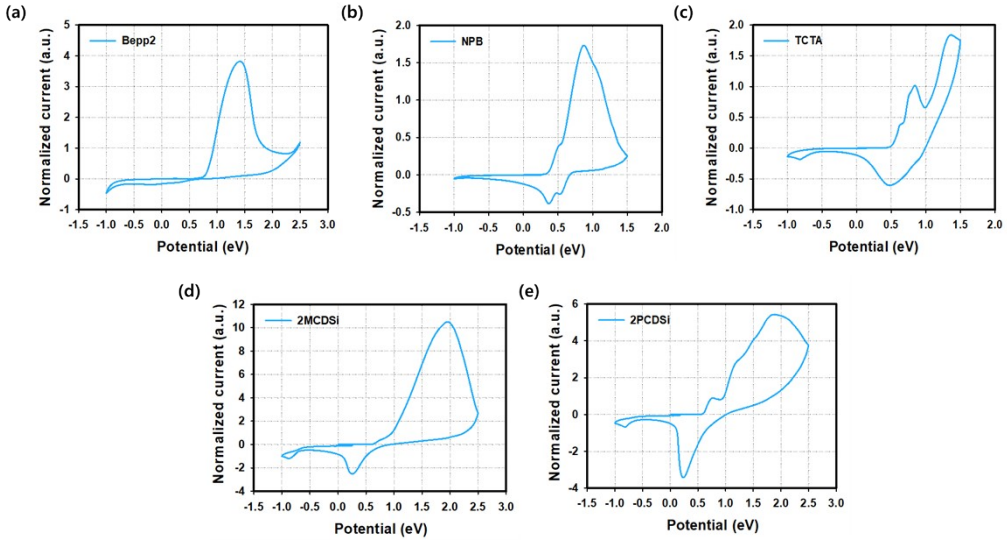


Figure S3. Cyclic-Voltammetry measurements for (a) Bepp2 (b) NPB (c) TCTA (d) 2MCDSi (e) 2PCDSi.

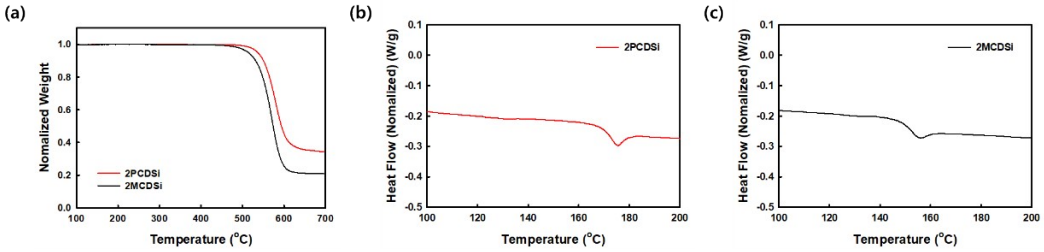


Figure S4. Thermal properties (a) TGA (b)&(C) DSC of 2PCDSi and 2MCDSi.

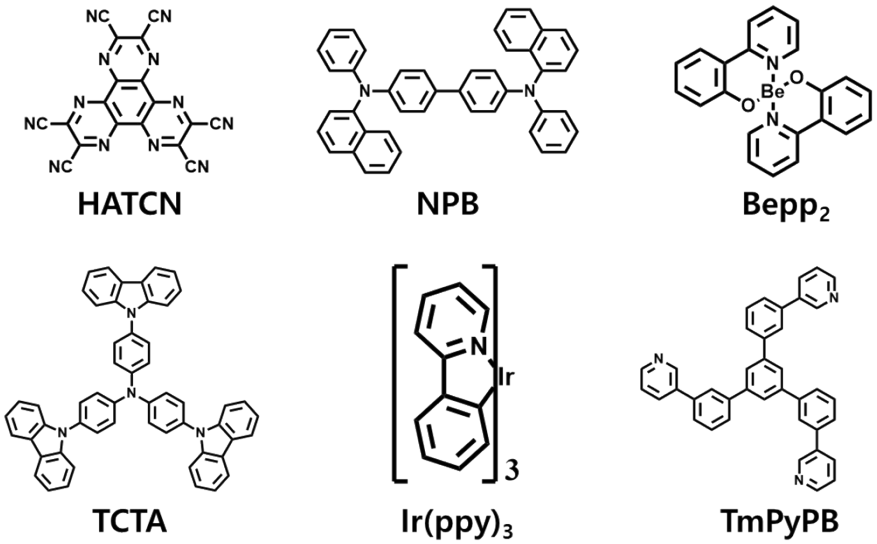


Figure S5. Molecular structures used for device fabrication.

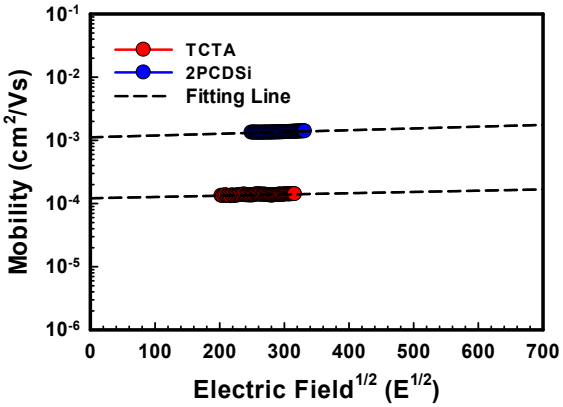


Figure S6. Space Charge Limited Current (SCLC) mobility of TCTA and 2PCDSi

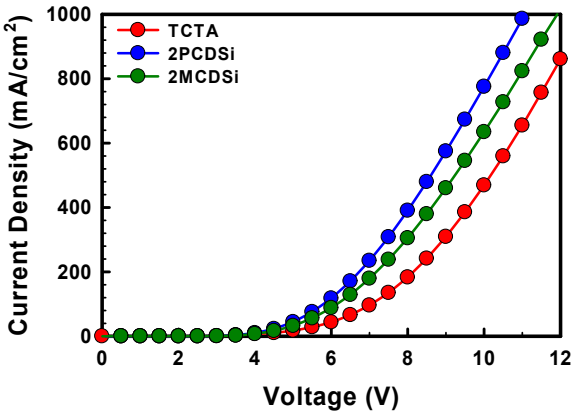


Figure S7. Hole Onley Device of TCTA, 2PCDSi and 2MCDSi

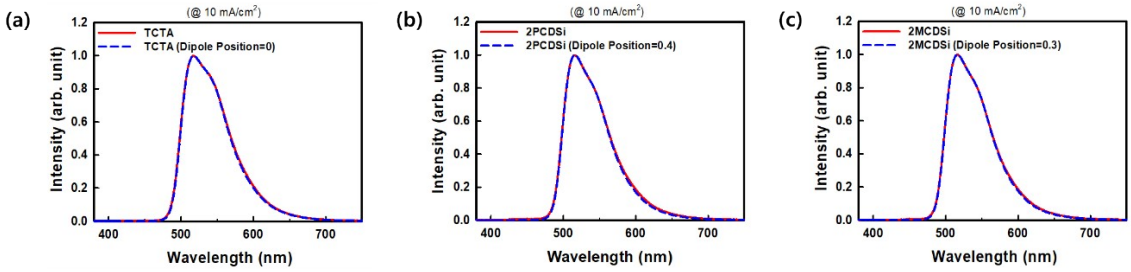


Figure S8. Fitted spectrum with TCTA, 2PCDSi, and 2MCDSi based OLED.

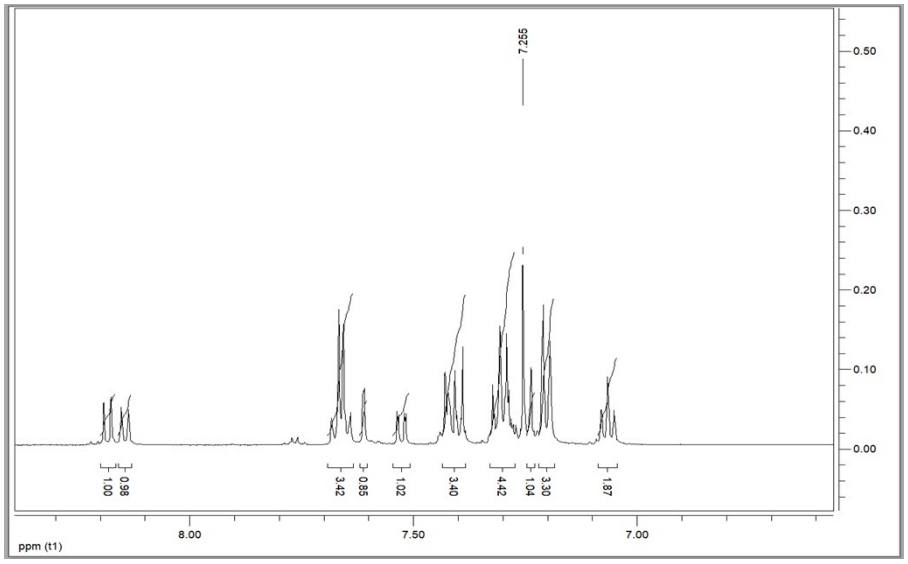


Figure S9. ^{1}H-NMR of 2PCDSi

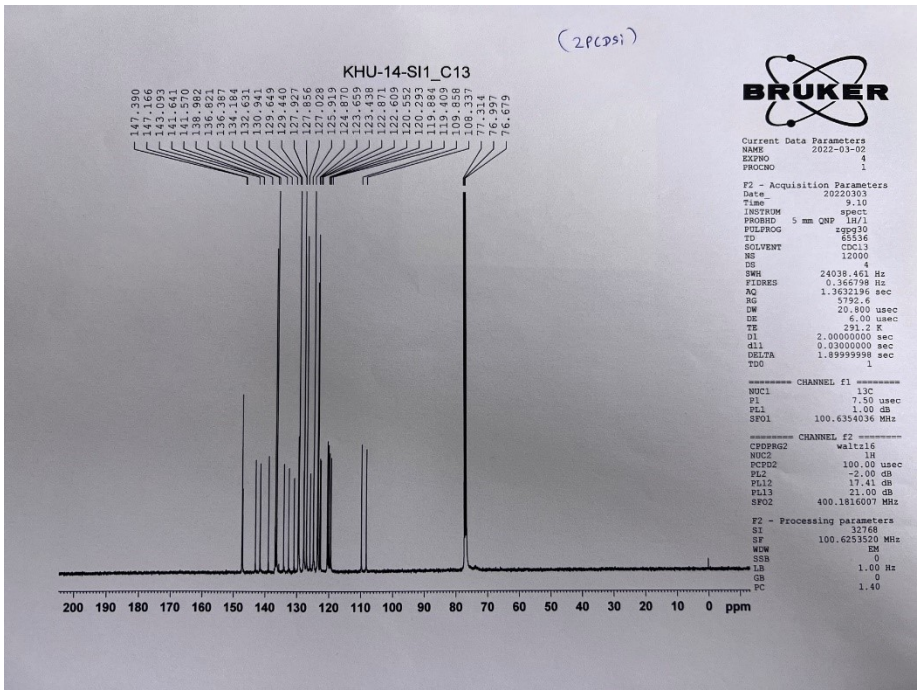


Figure S10. ^{13}C-NMR of 2PCDSi

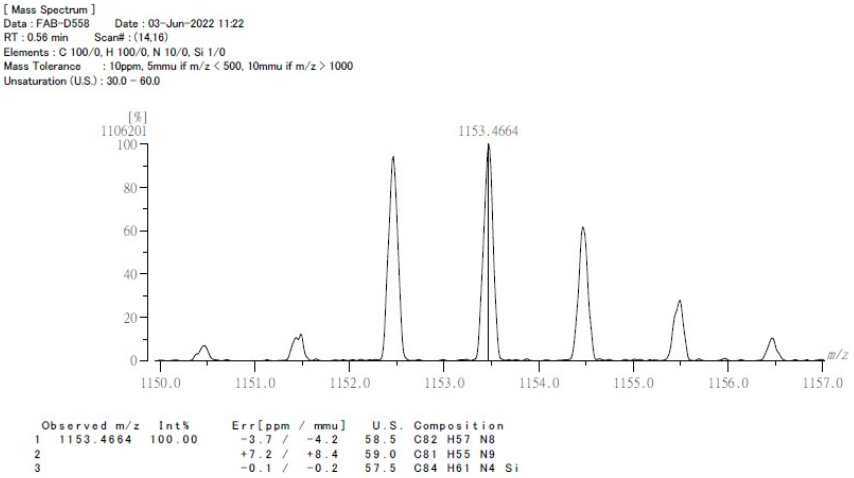


Figure S11. High Resolution Mass spectrum of 2PCDSi

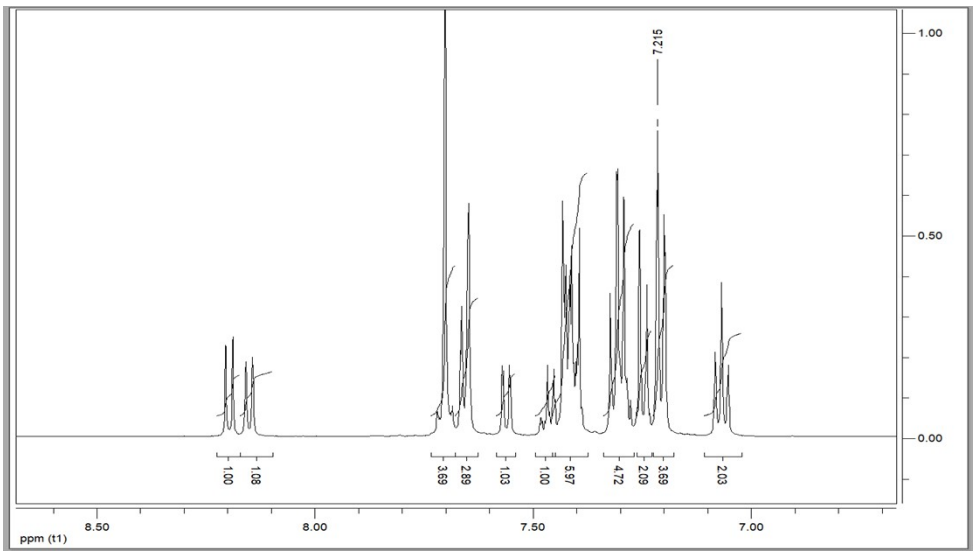


Figure S12. ^{1}H-NMR of 2MCDSi

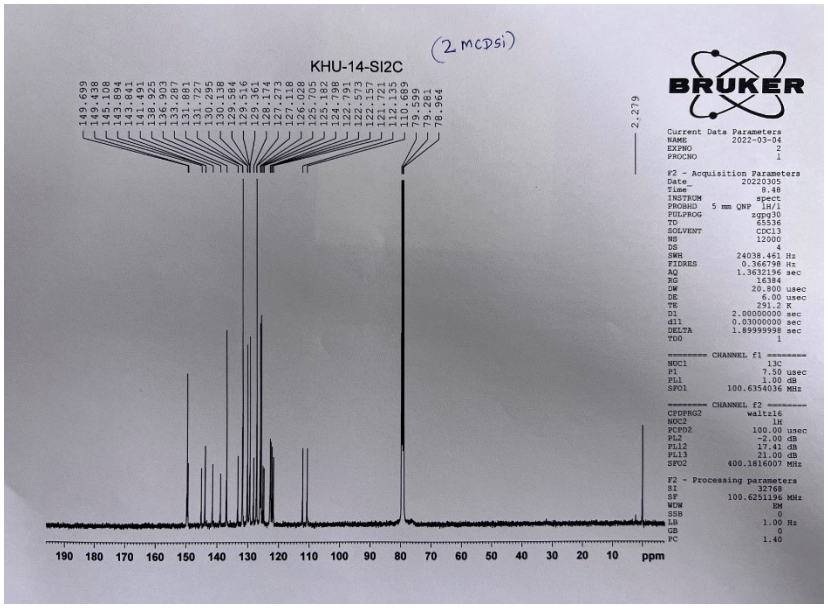


Figure S13. ^{13}C-NMR of 2MCDSi

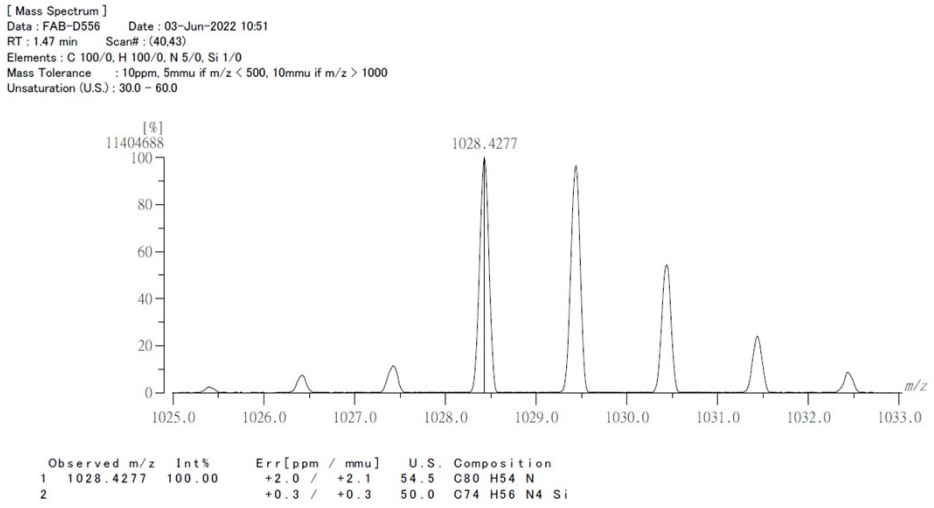


Figure S14. High Resolution Mass spectrum of 2MCDSi

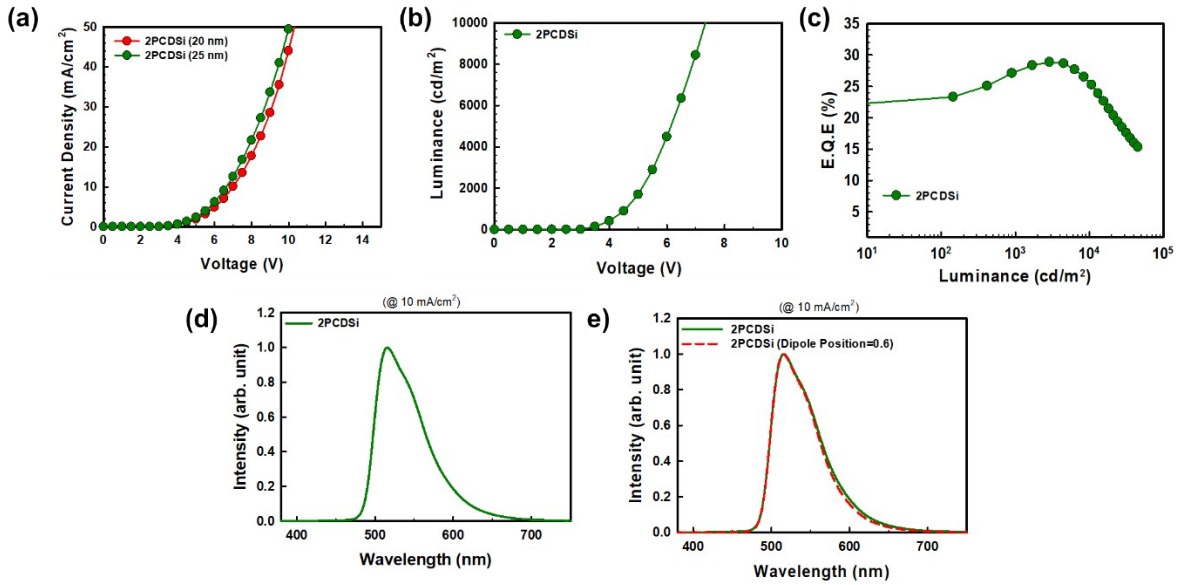


Figure S15. Increased 2PCDSi thickness. Device structure: ITO (50 nm)/ HATCN(7 nm)/ NPB (48nm)/ 2PCDSi (25nm)/ $Be(pp)_2$: 5.5 wt% $Ir(ppy)_3$ (25nm)/ TmPyPB (40nm)/ LiF (1.5nm)/ Al (100nm). (a) J (Current density)-V (Voltage), (b) L (Luminescence)-V (Voltage) (c) EQE (External Quantum Efficiency)-L (Luminescence) (d) EL spectra at 10mA/cm^2. (e), (f) Fitted spectrum with 2PCDSi based OLED.

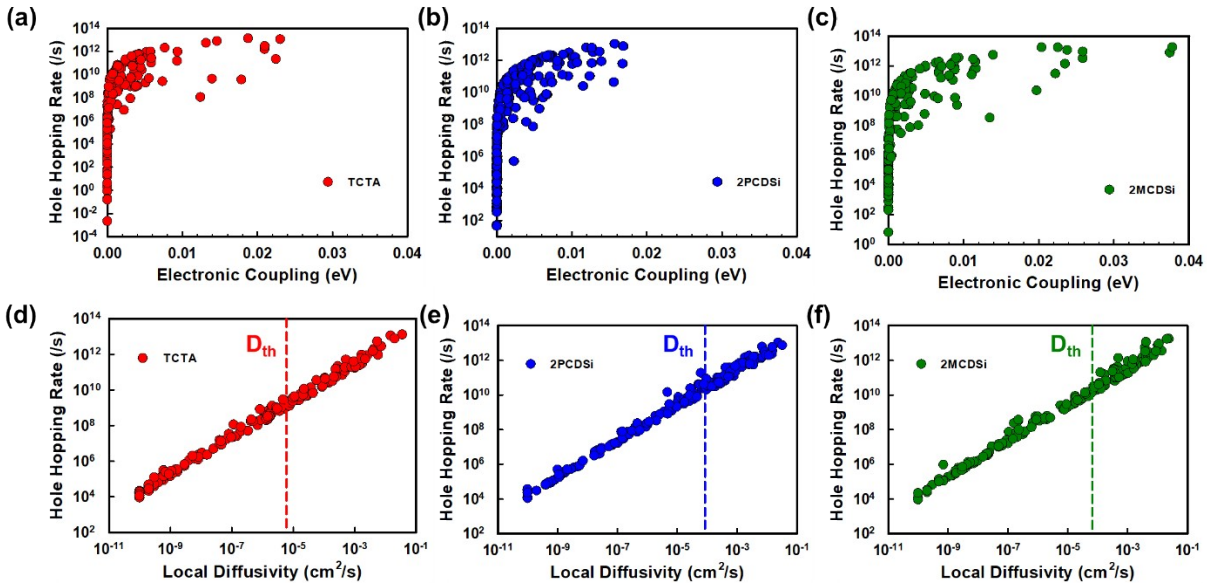


Figure S16. (a), (b), (c) hole hopping rate according to electronic coupling, (d), (e), (f) threshold diffusivity (D_{th}) that start to be attributed to hole diffusivity of TCTA, 2PCDSi, and 2MCDSi, respectively.

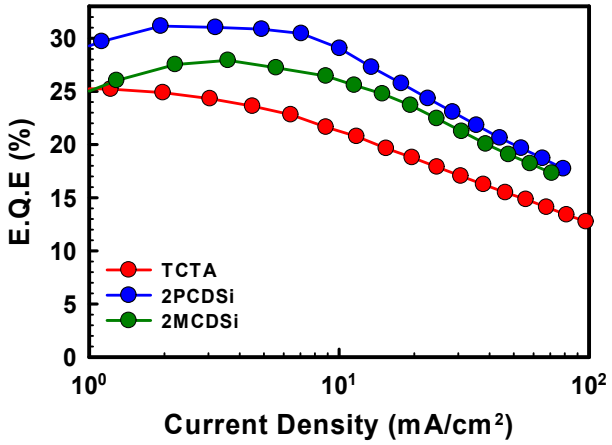


Figure S17. EQE (External Quantum Efficiency)- J (Current Density) plot of TCTA, 2PCDSi, and 2MCDSi.

Table S1. Calculated hole mobility through simulation ($\mu_{h,Simul}$) and Measured hole mobility through SCLC method ($\mu_{h,exp}$).

	$\mu_{h,Simul}$ (cm²/V)	$\mu_{h,exp}$ (cm²/V)
TCTA	2.46×10^{-4}	1.26×10^{-4}
2PCDSi	3.29×10^{-3}	1.12×10^{-3}
2MCDSi	2.81×10^{-3}	-