Supporting Information

A Robust Molecular Unit Nanogrid Servicing as Network Nodes via

Molecular Installing Technology

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General Procedures

Chemicals: All the solvents and reagents were purchased from commercial suppliers and used without further purification, unless noted otherwise. All products were purchased by flash column chromatography which was carried out with Kanto Silica Gel 60N (40-63 μ m). Spectrochemical-grade solvents were used for optical measurements. Palladiumacetate (Pd(OAc), tetra(triphenylphosphine)palladium (Pd(PPh_3)_4),

1,1'-bis(diphenylphosphino)ferrocene (dppf), 2-Bromo-9-fluorenone, bromobenzene and 9-hexylcarbazole were obtained from Aldrich Chemical Co. Borontrifluoride etherate, potassium carbonate, magnesium sulphate, chloroform, and toluene were purchased from Sinopharm Chemical Reagent Co, Ltd. without further purification. Dichloromethane were dried by anhydrous sodium under room temperature. THF and toluene were dried over sodium benzophenone ketyl anion radical and distilled under a dry nitrogen atmosphere immediately prior to use. 2-bromo-9-phenylfluoren-9-ol (1), 2-(4,4,5,5-tetramethyl- 1,3,2-dioxaborolan-2-yl)- 9-phenylfluoren-9-ol (2) were obtained according to the reported literatures¹.

Characterization: ¹H-NMR and ¹³C-NMR were recorded on a Bruker 400 MHz spectrometer in *d*-CDCl₃ with tetramethylsilane (TMS) as the interval standard. Mass spectra were recorded on a Shimadzu GC-MS 2010 PLUS. For the MALDI-TOF MS spectra, the spectra were recorded in reflective mode, and substrates were used. Molecular weights of the samples were measured by Gel permeation chromatography (GPC) on a Shimadzu LC-20A HPLC system equipped with 7911GP-502 and GPNXC columns. The calibration curves for GPC analysis were obtained using polystyrene standards with a low polydispersity. The sample (10 mg) was dissolved in THF (2 mL) and the solution was filtered through a membrane filter with a 0.45 µm pore size. Absorption spectra were measured with a Shimadzu UV-3150 spectrometer at 25 °C, and emission spectra were recorded on a Shimadzu RF-530XPC luminescence spectrometer upon excitation at the absorption maxima. Cyclic Voltammetry (CV) were conducted at room temperature on the

CHI660E system in a typical three-electrode cell with a platinum sheet working electrode, a platinum wire counter electrode, and a silver/silver nitrate (Ag/Ag⁺) reference electrode. All electrochemical experiments were carried out under a nitrogen atmosphere at room temperature and performed on the solution of the sample on a glassy carbon electrode measured in Bu4+PF6- (0.1 M)/acetonitrile at a sweeping rate of 0.1V/s. According to the redox onset potentials of the CV measurements, the highest occupied molecular orbital (HOMO)/lowest unoccupied energy levels (LUMO) of the materials are estimated based on the reference energy level of ferrocene (4.8 eV below the vacuum): HOMO/ LUMO = – ($E_{\text{ox/red}}$ - 0.09 V) +4.8 eV, where the value 0.09 V is the standard potential for ferrocene/ferrocenium vs Ag/Ag⁺. Thermogravimetric analyses (TGA) were conducted on a Shimadzu DTG-60H thermogravimetric analyzer under a heating rate of 10 °C /min. Differential scanning calorimetry (DSC) analyses were performed on a Shimadzu DSC-60A Instrument at a heating rate of 10 °C/min.

Theoretical Method: All the quantum-chemical calculations were performed using the Gaussian 09 program suite.² Non-covalent interactions (NCI) index is used to reveal weak bonding interactions and their intensities.³ The visualizing weak interactions in real space have been performed using Multiwfn 2.6 software and VMD by analyzing and ploting electrostatic potential on molecular surface.⁴

Experimental procedures and characterization

Synthesis of 2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9-phenylfluoren-9-ol (2)¹:



In a three-necked schlenk flask (150 mL), $\mathbf{1}^1$ (3.360 g, 10 mmol.), B_2Pin_2 (3.05 g, 12 mmol.), $Pd(OAc)_2$ (67 mg, 0.3 mmol.), KOAc (2.94 g, 30 mmol.), dppf (0.332 g, 0.6 mmol.) were added. The flask was evacuated and back-filled with nitrogen atmosphere over three times,

after which DMSO (30 mL) were injected into the flask through syringe. The reaction mixture was heated up to 80 °C and stirred for 8 h. The mixture was extracted three times with CH₂Cl₂ and the organic layer was dried over MgSO₄, filtered and the solvent was removed under reduced pressure. Purification by silica gel column chromatography (petroleum ether : CH₂Cl₂ = 20:1) to give **2** (3.03 g, 79%) as a pale yellow powder. ¹H NMR (400 MHz, CDCl₃) δ 7.84 (dd, *J* = 7.5, 0.8 Hz, 1H), 7.77 (s, 1H), 7.69 (t, *J* = 7.1 Hz, 2H), 7.41 – 7.36 (m, 3H), 7.36 (d, *J* = 1.3 Hz, 1H), 7.33 (s, 1H), 7.31 (s, 1H), 7.29 (q, *J* = 2.3 Hz, 1H), 7.24 (dt, *J* = 5.8, 2.0 Hz, 2H), 7.21 (d, *J* = 3.6 Hz, 1H), 2.47 (s, 1H), 1.31 (s, 13H). ¹³C NMR (100 MHz, CDCl₃) δ 149.73, 142.61, 139.33, 136.02, 129.07, 128.98, 128.22, 127.13, 125.52, 124.85, 120.52, 119.47, 83.86, 83.63, 25.03, 24.99, 24.75. GC-MS (m/z): calcd. For C₂₅H₂₅BO₃: 384.1 [M⁺]; Found: 384.0.

Synthesis of 9,9'-diphenyl-[2,2'-bifluorene]-9,9'-diol (I-1):



In a three-necked schlenk flask (150 mL), **1** (0.336 g, 1 mmol.), **2** (0.461 g, 1.2 mmol.), Pd(PPh₃)₄ (35 mg, 0.03mmol.) were added. The flask was evacuated and back-filled with nitrogen atmosphere over three times, after which degassed toluene (30 mL) and K₂CO₃ aqueous solution (2 M, 5 mL, 10 eq) were injected into the flask through syringe. The mixture was heated up to 90 °C and stirred for 24 h. The mixture was extracted three times with CH₂Cl₂ and the organic layer was dried over MgSO₄, filtered and the solvent was removed under reduced pressure. Purification by silica gel column chromatography (petroleum ether : CH₂Cl₂ = 1:1) to afford **I-1** (0.463 g, 90%) as a pale yellow powder. ¹H NMR (400 MHz, CDCl₃) δ 7.68 (t, *J* = 7.3 Hz, 1H), 7.57 (dd, *J* = 20.4, 12.4 Hz, 1H), 7.41 (d, *J* = 7.2 Hz, 1H), 7.36 (d, *J* = 7.5 Hz, 1H), 7.34 – 7.16 (m, 3H), 2.49 (s, 1H). ¹³C NMR

(100 MHz, CDCl₃) δ 151.18, 150.80, 143.04, 141.28, 139.12, 138.97, 129.17, 128.49, 128.31, 128.19, 127.29, 125.43, 124.78, 123.36, 120.42, 120.19, 83.68. MALDI-TOF-MS (m/z): calcd. For C₃₈H₂₆O₂: 514.1 [M⁺]; Found: 514.6.

Synthesis of 3-(2-bromo-9-phenyl-9H-fluoren-9-yl)-9-hexyl-9H-carbazole (3):



The compound was prepared by using **1** (0.336 g, 1 mmol.), 9-hexylcarbazole (0.301 g, 1.2 mmol), and BF₃·OEt₂ (0.4 mL, 1.5 mmol). The reaction mixture was stirred at rt for 24 h. The mixture was extracted three times with CH₂Cl₂ and the organic layer was dried over MgSO₄, filtered and the solvent was removed under reduced pressure. Purification by silica gel column chromatography (petroleum ether : CH₂Cl₂ = 10:1) to afford **3** (0.500 g, 88%) as a white powder. ¹H NMR (400 MHz, CDCl₃) δ 7.96 (d, *J* = 7.8 Hz, 1H), 7.91 (d, *J* = 1.0 Hz, 1H), 7.78 (d, *J* = 7.5 Hz, 1H), 7.66 (dd, *J* = 8.6, 4.9 Hz, 2H), 7.54 – 7.48 (m, 2H), 7.48 – 7.42 (m, 1H), 7.42 – 7.36 (m, 2H), 7.35 – 7.24 (m, 8H), 7.17 (dd, *J* = 10.9, 3.9 Hz, 1H), 4.25 (t, *J* = 7.3 Hz, 2H), 1.99 – 1.78 (m, 2H), 1.42 – 1.27 (m, 6H), 0.99 – 0.76 (m, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 154.10 , 151.86 , 146.07, 140.82, 139.45, 139.23, 139.02, 135.46, 130.64, 129.59, 128.40, 128.20, 127.59, 126.86, 126.43, 126.16, 125.69, 122.66, 121.56, 121.40, 120.46, 120.27, 119.61, 118.71, 108.66, 65.75, 43.19, 31.60 , 29.01, 27.01, 22.58, 14.07. GC-MS (m/z): calcd. For C₃₇H₂₂BrN: 569.1[M⁺]; Found: 569.6.

Synthesis of 9'-(9-hexyl-9*H*-carbazol-3-yl)-9,9'-diphenyl-9*H*,9'*H*-[2,2'-bifluoren]-9-ol (L-1):



In a three-necked schlenk flask (150 mL), 3 (0.569 g, 1 mmol.), 2 (0.461 g, 1.2 mmol.), $Pd(PPh_3)_4$ (35 mg, 0.03 mmol.) were added. The flask was evacuated and back-filled with nitrogen atmosphere over three times, after which degassed toluene (30 mL) and K₂CO₃ aqueous solution (2 M, 5 mL, 10 eq) were injected into the flask through syringe. The mixture was heated up to 90 °C and stirred for 2 days. The mixture was extracted three times with CH₂Cl₂ and the organic layer was dried over MgSO₄, filtered and the solvent was removed under reduced pressure. Purification by silica gel column chromatography (petroleum ether : $CH_2Cl_2 = 1:1$) to afford L-1 (0.433 g, 58%) as a pale yellow powder. ¹H NMR (400 MHz, CDCl₃) δ 7.93 (dd, J = 12.4, 8.9 Hz, 2H), 7.81 (dd, J = 7.7, 3.1 Hz, 2H), 7.67 (dd, J = 11.0, 3.6 Hz, 3H), 7.62 - 7.52 (m, 3H), 7.48 (d, J = 7.1 Hz, 1H), 7.43 - 7.30 (m, 10H), 7.27 (d, J = 7.9 Hz, 2H), 7.26 – 7.19 (m, 7H), 7.14 (dd, J = 15.4, 7.7 Hz, 1H), 4.23 (q, J = 7.6 Hz, 2H), 2.49 (s, 1H), 1.83 (dq, J = 14.8, 7.3 Hz, 2H), 1.32 (ddd, J = 11.6, 10.3, 5.7 Hz, 6H), 0.87 (d, J = 6.9 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 152.84, 152.47, 151.17, 150.79, 146.79, 143.18, 141.84, 140.88, 140.50, 139.77, 139.44, 138.71, 136.20, 129.21, 129.54 - 128.11, 127.87, 127.43, 127.11, 126.71, 126.67 - 126.14, 125.58, 124.90,123.58, 123.01–122.49, 120.39, 119.82, 118.71, 108.64 83.73, 65.83, 53.51, 43.20, 33.95, 32.06, 31.65, 30.45-28.53, 28.99-28.82, 28.99-28.68, 27.05, 22.73, 14.20. MALDI-TOF-MS (m/z): calcd. For C₅₆H₄₅NO: 747.3 [M⁺]; Found: 747.7.

Synthesis of 9,9'-bis(9-hexyl-9*H*-carbazol-3-yl)-9,9'-diphenyl-9*H*,9'*H*-2,2'-bifluorene (U-1):



The compound was prepared following the general procedures using **I-1** (0.514 g, 1 mmol.), 9-hexylcarbazole (0.753 g, 3.0 mmol.), and BF₃·OEt₂ (0.8 mL, 3.0 mmol.). The reaction mixture was stirred at rt under nitrogen for 24 h. The mixture was extracted three times with CH₂Cl₂ and the organic layer was dried over MgSO₄, filtered and the solvent was removed under reduced pressure. Purification by silica gel column chromatography (petroleum ether : $CH_2Cl_2 = 5:1$) to afford U-1 (0.931 g, 95%). The obtained white solid was recrystallized from CH₂Cl₂/hexane and yielded pure white solid. ¹H NMR (400 MHz, CDCl₃) δ 7.98 (m, 1H), 7.91 (m, 1H), 7.84 – 7.79 (m, 1H), 7.76 – 7.71 (m, 1H), 7.62 – 7.56 (m, 1H), 7.52 (d, J = 7.6 Hz, 1H), 7.46 – 7.31 (m, 3H), 7.31 – 7.18 (m, 3H), 7.14 (td, J = 7.1, 3.6 Hz, 1H), 4.23 (t, J = 7.2 Hz, 4H), 1.90 - 1.76 (m, 4H), 1.47 - 1.20 (m, 15H), 0.97 - 0.78 (m, 11H).NMR (100 MHz, CDCl₃) δ 152.61, 152.30, 146.79, 141.05, 140.97, 140.78, 139.79, 139.36, 136.24, 136.22, 128.81, 128.32, 128.29, 127.70, 127.43, 127.31, 127.22, 126.78, 126.73, 126.61, 126.43, 126.36, 126.32, 125.54, 125.06, 124.99, 122.77, 122.62, 122.59, 120.46, 120.39, 120.24, 119.70, 118.62, 108.60, 108.50, 65.70, 43.17, 31.60, 29.01, 27.01, 22.75, 22.59, 14.09, 14.08. MALDI-TOF-MS (m/z): calcd. For $C_{74}H_{64}N_2$: 980.5 [M⁺]; Found: 980.6.

Synthesis of 3-(2-bromo-9-phenyl-9H-fluoren-9-yl)-9-hexyl-9H-carbazole (4):



The compound was prepared following the general procedures using **1** (0.672 g, 2 mmol.), 3 (0.569 g, 1 mmol.), and BF₃·OEt₂ (0.4 mL, 1.5 mmol.). The reaction mixture was stirred at r.t. under nitrogen for 24 h. The mixture was extracted three times with CH₂Cl₂ and the organic layer was dried over MgSO₄, filtered and the solvent was removed under reduced pressure. Purification by silica gel column chromatography (petroleum ether : CH₂Cl₂ = 5:1) to afford **4** (0.800 g, 90%). The obtained white solid was recrystallized from CH₂Cl₂/hexane and yielded pure white solid. ¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, *J* = 8.3 Hz, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.60 (d, *J* = 3.3 Hz, 1H), 7.52 – 7.42 (m, 2H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.30 (t, *J* = 7.0 Hz, 1H), 7.28 – 7.17 (m, 7H), 4.18 (t, *J* = 7.3 Hz, 1H), 1.92 – 1.65 (m, 1H), 1.32 (d, *J* = 19.9 Hz, 5H). ¹³C NMR (100 MHz, CDCl₃) δ 154.04, 154.03, 151.83, 151.79, 146.09, 139.85, 139.84, 139.17, 139.16, 138.98, 138.96, 135.38, 135.37, 130.64, 129.57, 128.41, 128.15, 128.12, 127.57, 126.86, 126.40, 126.30, 126.25, 122.58, 122.54, 121.56, 121.39, 121.36, 120.25, 119.85, 119.79, 108.62, 108.59, 65.72, 65.71, 43.23, 31.57, 29.75, 28.99, 26.97, 22.55, 14.07. MALDI-TOF-MS (m/z): calcd. For C₅₆H₄₃Br₂N: 889.1 [M⁺]; Found: 888.9.

Synthesis of

9',9'''-(9-hexyl-9*H*-carbazole-3,6-diyl)bis(9,9'-diphenyl-9*H*,9'*H*-[2,2'-bifluoren]-9-ol) (U-2):



In a three-necked schlenk flask (150 mL), **4** (0.889 g, 1 mmol.), **2** (1.152 g, 3 mmol.), Pd(PPh₃)₄ (70 mg, 0.06mmol.) were added. The flask was evacuated and back-filled with nitrogen atmosphere over three times, after which degassed toluene (30 mL) and K₂CO₃ aqueous solution (2M, 5 mL, 10 eq) were injected into the flask through syringe. The

mixture was heated up to 90 °C and stirred for 2 days. The mixture was extracted three times with CH₂Cl₂ and the organic layer was dried over MgSO₄, filtered and the solvent was removed under reduced pressure. Purification by silica gel column chromatography (petroleum ether : CH₂Cl₂ = 1:1) to afford **U-2** (0.634 g, 51%) as a white powder. ¹H NMR (400 MHz, CDCl₃) δ 7.83 (d, *J* = 10.1 Hz, 2H), 7.77 (t, *J* = 7.2 Hz, 4H), 7.70 – 7.58 (m, 6H), 7.56 – 7.46 (m, 6H), 7.45 – 7.30 (m, 12H), 7.26 (s, 4H), 7.26 – 7.25 (m, 1H), 7.24 (d, *J* = 2.7 Hz, 6H), 7.23 – 7.14 (m, 14H), 4.21 – 4.08 (m, 2H), 2.52 (d, *J* = 19.1 Hz, 1H), 2.46 (s, 1H), 1.83 – 1.71 (m, 2H), 1.31 – 1.21 (m, 6H), 0.86 – 0.80 (m, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 152.78, 152.48, 151.05, 150.74, 146.65, 143.10, 141.86, 140.36, 139.63, 139.30, 138.77–138.42, 136.06–135.63, 129.18, 128.30, 127.76, 127.33, 127.17–126.86, 126.49, 125.46, 124.85, 123.47, 122.87–122.29, 120.27, 119.99–119.26, 108.46, 83.66, 65.71, 43.19, 31.55, 29.74, 28.97, 26.96, 22.53, 14.04. MALDI-TOF-MS (m/z): calcd. For C₉₄H₆₉NO₂: 1244.5 [M⁺]; Found: 1244.1.

Synthesis of Grid-1with L-1:



The compound was prepared by using **L-1** (0.224 g, 0.3 mmol), BF₃·OEt₂ (0.4 ml, 1.5 mmol) was diluted together with CH₂Cl₂ then dropwise. The reaction mixture was stirred at rt under nitrogen for 24 h. The mixture was extracted three times with CH₂Cl₂ and the organic layer was dried over MgSO₄, filtered and the solvent was removed under reduced pressure. Purification by silica gel column chromatography (petroleum ether : CH₂Cl₂ = 2:1) to afford **Grid** (0.306g, 21%) as a white powder. ¹H NMR (400 MHz, CDCl₃) δ 7.90 (d, *J* = 7.5 Hz, 1H), 7.80 (s, 1H), 7.66 (dd, *J* = 16.9, 7.7 Hz, 3H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.38 – 7.30 (m,

3H), 7.07 (d, J = 11.5 Hz, 7H), 4.19 (d, J = 7.1 Hz, 4H), 1.79 (d, J = 7.1 Hz, 4H), 1.38 – 1.25 (m, 6H), 0.87 (dd, J = 12.4, 5.8 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 152.12, 141.94, 140.34, 139.44, 138.53, 135.63, 128.19, 127.91, 127.68, 127.54, 126.39, 126.20, 120.59, 119.78, 65.41, 43.29, 31.54, 29.72, 26.95, 22.55, 14.03. MALDI-TOF-MS (m/z): calcd. For C₁₁₂H₈₆N₂: 1458.6 [M+]; Found: 1458.7.

Synthesis of Grid-1



The compound was prepared by using **I-1** (0.514 g, 1 mmol.), 9-hexylcarbazole (0.251 g, 1 mmol.) and BF₃·OEt₂ (1.6 mL, 6 mmol) was diluted together with CH₂Cl₂ then dropwise,. The reaction mixture was stirred at rt under nitrogen for 24 h. The mixture was extracted three times with CH₂Cl₂ and the organic layer was dried over MgSO₄, filtered and the solvent was removed under reduced pressure. Purification by silica gel column chromatography (petroleum ether: CH₂Cl₂ = 2:1) to afford **Grid** (0.146 g, 10%) as a white powder.

Synthesis of Grid-1with U-1:



The compound was prepared by using **I-1** (0.102 g, 0.2 mmol.), **U-1** (0.196 g, 0.2 mmol.) and $BF_3 \cdot OEt_2$ (0.3 mL, 1.2 mmol) was diluted together with CH_2Cl_2 then dropwise. The

reaction mixture was stirred at rt under nitrogen for 24 h. The mixture was extracted three times with CH_2Cl_2 and the organic layer was dried over MgSO₄, filtered and the solvent was removed under reduced pressure. Purification by silica gel column chromatography (petroleum ether : $CH_2Cl_2 = 2:1$) to afford **Grid** (0.062 g, 4.3%) as a white powder.

Synthesis of Grid-1with U-2:



The compound was prepared by using U-2 (0.124 g, 0.1 mmol.), 9-hexyl-9H-carbazole (0.025 g, 0.1 mmol.) and BF₃·OEt₂ (0.16 ml, 0.6 mmol) was diluted together with CH₂Cl₂ then dropwise. The reaction mixture was stirred rt under nitrogen for 24 h. The mixture was extracted three times with CH₂Cl₂ and the organic layer was dried over MgSO₄, filtered and the solvent was removed under reduced pressure. Purification by silica gel column chromatography (petroleum ether : CH₂Cl₂ = 2:1) to afford **Grid** (0.087 g, 6.0%) as a white powder.

OLED based on Grid



Fig. 1 (a) The schematic illustration of the OLED; (b) Energy level diagrm of OLED; (c) The EL spectra of **Grid**; (d) L-V and LE-V characteristics of the device prepared from **Grid**.

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MALDI-TOF-MS of compounds:



Fig. 2 MALDI-TOF-MS spectra of I-1







Fig. 4 MALDI-TOF-MS spectra of L-1



Fig. 5 MALDI-TOF-MS spectra of U-1



Fig. 6 MALDI-TOF-MS of 4







Fig. 8 MALDI-TOF-MS of Grid

GPC spectrum and crude product of Grid



Fig. 9 GPC spectrum of Grid and crude product of Grid

Standard potential for ferrocene/ferrocenium vs Ag/Ag⁺



Fig. 10 Cyclic voltammograms of ferrocene/ferrocenium vs Ag/Ag⁺

compound	Oxidation potential	Reduction potential	HOMO	LUMO
Grid	0.87 eV	-2.51 eV	5.58 eV	-2.20 eV

Table 1 The HOMO and LUMO en	nergy levels of Grid
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¹H and ¹³C NMR spectra of the compounds







SI-22







