Supporting Information

Novel Deep Blue Hot Exciton Material for High-Effeciency Nondoped Organic Light-Emitting Diode

Pei Xu, a Lei Xu, a Yuyu Pan, c Dezhi Yang, a Zetong Ma, a Xianfeng Qiao, a Dehua Hu, *a,b Dongge Ma, a and Yuguang Ma* a

a State Key Laboratory of Luminescent Materials and Devices, South China University of Technology, Guangzhou, 510640, P. R. China

b School of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou 510006, China.

c Shenyang Univ Technol, Sch Petrochem Engn, 30 Guanghua St, Liaoyang 111003, P. R. China

E-mail: msdhhu@scut.edu.cn; ygma@scut.edu.cn

Contents

S1. Synthesis General

S2. Supplementary Thermal and Electrochemical Properties

S3. Supplementary Theoretical Calculations

S4. Supplementary Photophysical Properties

S5. Supplementary Electroluminescence Performances

S6. Supplementary Mechanism Study
S1. Synthesis General

The $^1$H NMR spectra was recorded on a Bruker AVANCE 500 spectrometer at 500 MHz, using tetramethylsilane (TMS) as the internal standard and CDCl$_3$ as the solvent. The matrix- assisted laser desorption ionization time-of-flight (MALDI-TOF) mass spectrum was measured using an AXIMA-CFRTM plus instrument.

$^1$H NMR (500 MHz, Chloroform-d) $\delta$ 8.04 (t, $J$ = 1.7 Hz, 1H), 7.93 (d, $J$ = 6.5 Hz, 2H), 7.91 - 7.86 (m, 2H), 7.78 - 7.70 (m, 6H), 7.66 - 7.61 (m, 2H), 7.59 - 7.53 (m, 2H), 7.47 (t, $J$ = 7.6 Hz, 4H), 7.42 - 7.35 (m, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 143.48, 140.89, 139.67, 138.65, 136.93, 133.66, 131.30, 131.26, 128.81, 128.40, 127.88, 126.65, 126.28, 125.03, 124.77, 124.39, 124.22, 117.89, 110.62.

MALDI-TOF-MS (m/z): calcd for C$_{39}$H$_{25}$N, 507.20; found, 507.28 [M+].

Figure S1. $^1$H-NMR Spectrum of MACN in CDCl$_3$. 
Figure S2. Mass Spectrum (M+H+) of MACN.

S2. Supplementary Thermal and Electrochemical Properties

Figure S3. (a) TGA and DSC curves (inset) of MACN. (b) Electrochemical CV curves of MACN.

S3. Supplementary Theoretical Calculations

<table>
<thead>
<tr>
<th></th>
<th>Singlets</th>
<th>Triplet</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Hole</td>
<td>Particle</td>
</tr>
<tr>
<td>(S_0 \rightarrow S_1)</td>
<td>98.60%</td>
<td>(96.89%)</td>
</tr>
<tr>
<td>(S_0 \rightarrow S_2)</td>
<td>50.12%</td>
<td>(57.21%)</td>
</tr>
<tr>
<td>(S_0 \rightarrow S_3)</td>
<td>99.84%</td>
<td>(64.01%)</td>
</tr>
</tbody>
</table>
S4. Supplementary Photophysical Properties

Figure S4. The NTO transition character of the first five singlet and triplet states.

S5. Supplementary Electroluminescence Performances

To evaluate the transporting properties of this material, single-carrier devices were fabricated with structure of ITO/NPB (10 nm)/MACN (80nm)/NPB (10 nm)/Al for hole-only device and ITO/TPBi (10 nm)/MACN (80 nm)/TPBi (10 nm)/LiF /Al for electron-only device. NPB and TPBi are used to prevent electron and hole injection from the cathode and anode, respectively. As the voltage increased, the current becomes space-charge limited with a nearly quadratic dependence on voltage. The hole and electron mobilities were calculated from the slope of the J^{1/2}-V curves to be 1.47×10^{-12} cm^2 V^{-1}s^{-1} and 6.13×10^{-7} cm^2 V^{-1} s^{-1}, respectively, indicating that imbalance of carrier recombination may be the reason for limiting the EQE of devices based on MACN.
**Figure S6.** Current density versus voltage characteristics of the hole-only and electron-only devices.

**Figure S7.** (a) J-V-L curves of the devices. (b) CE-L-PE characteristics. (c) L-EQE curves. (d) The EL spectra.

**Table S2.** Device performances of MACN OLEDs with different structures

<table>
<thead>
<tr>
<th>Device</th>
<th>$V_{on}$ (V)</th>
<th>$L_{max}$ (cd m$^{-2}$)</th>
<th>$CE_{max}$ (cd A$^{-1}$)</th>
<th>EQE$_{max}$ (%)</th>
<th>PE$_{max}$ (lm W$^{-1}$)</th>
<th>EL peak (nm)</th>
<th>CIE (x,y)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>3.8</td>
<td>3942</td>
<td>4.99</td>
<td>7.51</td>
<td>3.14</td>
<td>436</td>
<td>(0.154,0.075)</td>
</tr>
<tr>
<td>B</td>
<td>4</td>
<td>2682</td>
<td>3.56</td>
<td>5.31</td>
<td>2.94</td>
<td>436</td>
<td>(0.155,0.075)</td>
</tr>
<tr>
<td>C</td>
<td>3</td>
<td>3236</td>
<td>3.21</td>
<td>4.71</td>
<td>1.99</td>
<td>438</td>
<td>(0.153,0.75)</td>
</tr>
</tbody>
</table>

Device A: ITO/ PEDOT: PSS (40 nm)/TCTA (40 nm)/MACN (20 nm)/TPBi (30 nm)/LiF/Al

Device B: ITO/P PEDOT: PSS (40 nm)/TCTA (40 nm)/MACN (20 nm)/TmPyPb (30 nm)/LiF/Al
Device C: ITO/ PEDOT: PSS (40 nm) /TAPC (20 nm) /TCTA (30 nm)/MACN (20 nm)/TPBi (30 nm)/LiF/Al

Figure S8. Variable-angle PL measurements of MACN film. Θ, orientation factors. For fully horizontal dipoles, Θ equals 100% and isotropic dipole orientation, Θ equals 67%.

S6. Supplementary Mechanism Study

Figure S9. (a) Transient absorption spectra of the pristine PtOEP solution. (b) Transient absorption spectra of the MACN & PtOEP solution.

Figure S10. (a) Top: the delayed emission spectrum of the MACN & BP solution; middle: the phosphorescence spectrum of BP. The fluorescence spectrum of MACN at 77 K appears at the
bottom. In the mixed solution, the concentration of the ketones was $10^{-5}$ M, and the concentration of MACN was $10^{-4}$ M. The excitation wavelength was 280 nm. (b) The PL decay spectra of the MACN and MACN& IDO solutions at room temperature.