Supporting Information for

“Multi-Carbazole Derivatives: New Dyes for Highly Efficient Dye-Sensitized Solar Cells”

By Hua Lai,¹ Jia Hong,¹ Ping Liu,² Chao Yuan,¹ Yuxue Li, *¹ and Qiang Fang*¹,³

¹Key Laboratory of Organofluorine Chemistry, State Key Laboratory of Organometallic Chemistry and Laboratory for Polymer Materials, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai 200032, PR China
²College of Materials and Engineering, South China University of Technology, Guangzhou 510640, PR China
³Shanghai Advanced Research Institute, Chinese Academy of Sciences, 99 Haike Road, Zhangjiang Hi-Tech Park, Pudong, Shanghai 201203, PR China

*Corresponding authors. E-mail: qiangfang@mail.sioc.ac.cn, Tel & Fax: (+86) 21-54925337

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1. Detailed Characterization

![H NMR spectrum of 6 (300 MHz, CDCl₃). The peak with asterisk is attributed to CHCl₃ and the peaks with square are attributed to H₂O or impurities, respectively.]

![13C NMR spectrum of 6 (100 MHz, CDCl₃). The peak with asterisk is attributed to CHCl₃.]

**Figure S1.** $^1$H NMR spectrum of 6 (300 MHz, CDCl₃). The peak with asterisk is attributed to CHCl₃ and the peaks with square are attributed to H₂O or impurities, respectively.

**Figure S2.** $^{13}$C NMR spectrum of 6 (100 MHz, CDCl₃). The peak with asterisk is attributed to CHCl₃.
Figure S3. $^1$H NMR spectrum of 8 (300 MHz, CDCl$_3$). The peak with asterisk is attributed to CHCl$_3$ and the peaks with square are attributed to H$_2$O or impurities, respectively.
**Figure S4.** $^{13}$C NMR spectrum of 8 (100 MHz, CDCl$_3$). The peak with asterisk is attributed to CHCl$_3$ and the peaks with square are attributed to impurities, respectively.

**Figure S5.** $^1$H NMR spectrum of 9 (300 MHz, CDCl$_3$). The peak with asterisk is attributed to CHCl$_3$ and the peaks with square are attributed to H$_2$O or impurities, respectively.

**Figure S6.** $^{13}$C NMR spectrum of 9 (100 MHz, CDCl$_3$). The peak with asterisk is attributed to CHCl$_3$ and the peaks with square are attributed to impurities, respectively.
Figure S7. $^1$H NMR spectrum of 2C (300 MHz, DMSO-d6). The peak with asterisk is attributed to DMSO and the peak with square are attributed to H$_2$O, respectively.

Figure S8. $^{13}$C NMR spectrum of 2C (100 MHz, DMSO-d6). The peak with asterisk is attributed to DMSO.
Figure S9. $^1$H NMR spectrum of 3C (300 MHz, DMSO-$d_6$). The peak with asterisk is attributed to DMSO and the peak with square is attributed to H$_2$O, respectively.

Figure S10. $^{13}$C NMR spectrum of 3C (100 MHz, DMSO-$d_6$). The peak with asterisk is attributed to DMSO.
**Figure S11.** $^1$H NMR spectrum of 4C (300 MHz, DMSO-$d_6$). The peak with asterisk is attributed to DMSO and the peak with square is attributed to H$_2$O, respectively.

**Figure S12.** $^{13}$C NMR spectrum of 4C (100 MHz, DMSO-$d_6$). The peak with asterisk is attributed...
DMSO.

**Figure S13.** Mass spectrum of 6.

**Figure S14.** Mass spectrum of 8.
Figure S15. Mass spectrum of 9.

Figure S16. Mass spectrum of 2C.
**Figure S17.** Mass spectrum of 3C.

**Figure S18.** Mass spectrum of 4C.

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2. Optical properties of the dyes

![Normalized UV-vis spectra of 2C-4C in THF and on TiO₂.](image)

**Figure S19.** Normalized UV-vis spectra of 2C-4C in THF and on TiO₂.
Table S1. The maximum and onset absorption wavelength for 2C-4C in THF and on TiO$_2$

<table>
<thead>
<tr>
<th>Dyes</th>
<th>In THF$^a$</th>
<th></th>
<th>On TiO$_2$$^b$</th>
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<tr>
<td></td>
<td>$\lambda_{\text{max}}$ (nm)</td>
<td>$\lambda_{\text{onset}}$ (nm)</td>
<td>$\lambda_{\text{max}}$ (nm)</td>
<td>$\lambda_{\text{onset}}$ (nm)</td>
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<tr>
<td>4C</td>
<td>456</td>
<td>530</td>
<td>460</td>
<td>565</td>
</tr>
</tbody>
</table>

$^a$ In THF solution (10$^{-5}$ M). $^b$ On TiO$_2$ (12 μm) films which were immersed into 1.5×10$^{-4}$ M solution of these dyes in THF for 12 h.

Figure S20. Normalized PL spectra of the dyes in THF.
3. The theory estimation of HOMO and LUMO for the dyes

<table>
<thead>
<tr>
<th>HOMO</th>
<th>LUMO</th>
</tr>
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<tbody>
<tr>
<td>2C</td>
<td></td>
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<tr>
<td>3C</td>
<td></td>
</tr>
<tr>
<td>4C</td>
<td></td>
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</table>

Figure S21. Frontier molecular orbital of the HOMO and LUMO calculated with DFT. (Density functional theory (DFT) calculations were conducted by using the B3LYP hybrid functional for the geometry optimizations. The molecular orbital levels of HOMO and LUMO were achieved with the 6-31G(d) basis set implemented in the Gaussian 03 package\(^1\))

Reference