Supporting Information

Fast Predictions of Exciton Diffusion Length in Organic Materials

Leonardo Evaristo de Sousa,†‡ Fernando Teixeira Bueno,† Geraldo Magela e Silva,† Demétrio Antônio da Silva Filho,† and Pedro Henrique de Oliveira Neto*,†

†Institute of Physics, University of Brasilia, Brasilia, Brazil
‡Theoretical and Structural Chemistry Group, State University of Goias, Anapolis, Brazil

E-mail: pedrohenrique@unb.br

Parameters

Table 1 shows refractive indices and emission lifetimes used to calculate each molecule’s Förster radius. Emission lifetimes are obtained from the simulated emission spectra.

Spectra

The following figures show the absorption and emission spectra of all the molecules analyzed in the work.
Table 1: Refractive indexes and radiative lifetimes for all molecules studied in this work. The latter are obtained from emission spectrum simulations.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>n</th>
<th>Lifetime (ns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Naphthalene</td>
<td>1.6</td>
<td>8.5</td>
</tr>
<tr>
<td>Anthracene</td>
<td>1.6</td>
<td>18.5</td>
</tr>
<tr>
<td>Tetracene</td>
<td>1.8</td>
<td>30.9</td>
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<tr>
<td>Pentacene</td>
<td>1.8</td>
<td>61.5</td>
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<tr>
<td>P6P</td>
<td>1.7</td>
<td>0.3</td>
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<td>6T</td>
<td>1.9</td>
<td>0.6</td>
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<td>AlQ3</td>
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<td>20786</td>
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<tr>
<td>DIP</td>
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<td>99.6</td>
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<tr>
<td>Dibromonaphtalene</td>
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<td>mCP</td>
<td>1.5</td>
<td>21.1</td>
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<tr>
<td>Pyrene</td>
<td>1.8</td>
<td>2.2</td>
</tr>
</tbody>
</table>

Figure 1: Emission and absorption spectra for sexithiophene (6T).
Figure 2: Emission and absorption spectra for tris-(8-hydroxyquinoline)aluminum (AlQ3).
Energy (eV)

Anthracene ($\text{C}_{14}\text{H}_{10}$)

Figure 3: Emission and absorption spectra for anthracene
Figure 4: Emission and absorption spectra for 1,4-Dibromonaphtalene.
Figure 5: Emission and absorption spectra for 1,3-Bis(N-carbazolyl)benzene (mCP)
Figure 6: Emission and absorption spectra for Naphthalene
Figure 7: Emission and absorption spectra for para-hexaphenyl (P6P)
Figure 8: Emission and absorption spectra for pentacene.
Figure 9: Emission and absorption spectra for pyrene.
Figure 10: Emission and absorption spectra for tetracene.
Figure 11: Emission and absorption spectra for DIP.