Supporting Information

Ligand mediated excited state carrier relaxation dynamics of Cd$_{1-x}$Zn$_x$Se$_{1-y}$S$_y$
NCs derived from bile salts

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1. ICP-OES analysis

Table 1. Characterization of CdDCh$_2$ and ZnDCh$_2$ by Inductively-coupled Plasma Optical Emission Spectrometry (ICP-OES) and C, H elemental analysis

<table>
<thead>
<tr>
<th>Sample</th>
<th>ICP-OES</th>
<th>Elemental analysis (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CdDCh$_2$</td>
<td>Calculated for C$<em>{48}$H$</em>{78}$O$_8$Cd</td>
<td>% of Cd=12.6</td>
</tr>
<tr>
<td></td>
<td>Experimental % of Cd=13.2</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Calculated for C$<em>{48}$H$</em>{78}$O$_8$Cd,3H$_2$O</td>
<td>C=60.71, H=8.92</td>
</tr>
<tr>
<td></td>
<td>Experimental C=60.87, H=8.88</td>
<td></td>
</tr>
<tr>
<td>ZnDCh$_2$</td>
<td>Calculated for C$<em>{48}$H$</em>{78}$O$_8$Zn</td>
<td>% of Zn=7.7</td>
</tr>
<tr>
<td></td>
<td>Experimental % of Zn=8.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Calculated for C$<em>{48}$H$</em>{78}$O$_8$Zn,3H$_2$O</td>
<td>C=63.88, H=9.28</td>
</tr>
<tr>
<td></td>
<td>Experimental C=63.12, H=8.60</td>
<td></td>
</tr>
</tbody>
</table>

Sample preparation of ICP-OES analysis: A known weight of CdDCh$_2$ (2-5 mg) (or, ZnDCh$_2$) was digested with c. H$_2$SO$_4$ and 30% H$_2$O$_2$ (0.75 mL and 0.18 mL, respectively) upon heating at 130 °C for 45 min. The sample solution was cooled to room temperature and diluted to 50 mL with distilled water to prepare the unknown sample solution. The concentration was found out from a standard calibration curve.

2. Thermogravimetric analysis (TGA)

Fig. S1. Thermogravimetric analysis curves of (a) CaDCh$_2$ and (b) ZnDCh$_2$. 
3. **Field emission transmission electron microscopy (FETEM).**

TEM images were recorded on JEOL 2100F. For TEM imaging NC dispersion in chloroform was cast on a carbon-coated copper grid (400 square mesh) and followed by high vacuum drying. The operating voltage for FETEM was 200 KV.

4. **UV-visible, Fluorescence, photoluminescent quantum yield and time resolve spectroscopy.**

Absorption and Fluorescence measurements were carried out on a Shimadzu UV-3600 spectrophotometer and Varian Cary Eclipse fluorescence spectrometer. UV-visible absorption and emission spectra of the NCs were recorded on a UV-Vis spectrophotometer and emission at room temperature using quartz cuvette. The photoluminescent quantum yields were recorded on Edinburgh Instruments FLS980 fluorescence spectrometer equipped with an integrating sphere. A light emitting diode (FLSP920) at 405 nm was used as excitation source. The instrument response function was measured by scattering the exciting light of aqueous milk powder. Fitting and analysis was performed using Origin8 and Xmgrace software.

5. The average life time ($<\tau>$) values of the NCs sample were estimated using following equation:

$$<\tau> = \frac{\sum A_i \tau_i^2}{\sum A_i \tau_i}; i = 1,2,3$$
6. Additional TEM images.

Fig S2. (a, b) TEM images and (c, d) STEM-EDS area mapping of composition of HDA capped Cd_{1-x}Zn_xSe_{1-y}S_y NCs.
Fig S3. TEM images of OA capped Cd$_{1-x}$Zn$_x$Se$_{1-y}$S$_y$ NCs.
Fig S4. (a, b) TEM images and (c, d) STEM-EDS line mapping of composition of TOPO capped Cd$_{1-x}$Zn$_x$Se$_{1-y}$S$_y$ NCs.
7. STEM mapping and energy-dispersive X-ray spectra (EDS) of HDA, OA and TOPO capped NCs.

Fig S5. STEM area mapping and EDS of composition of HDA capped Cd\textsubscript{1-x}Zn\textsubscript{x}Se\textsubscript{1-y}S\textsubscript{y} NCs.
Fig S6. STEM area mapping and EDS of composition of OA capped Cd$_{1-x}$Zn$_x$Se$_{1-y}$S$_y$ NCs.
Fig S7. STEM area mapping and EDS of composition of TOPO capped Cd$_{1-x}$Zn$_x$Se$_{1-y}$S$_y$ NCs.
8. Emission and time resolved spectra of HDA, OA and TOPO capped orange emitting NCs:

Fig S8. (a) photoluminescence and (b) fluorescence lifetime (UV excitation at 400 nm) spectra of HDA, OA and TOPO capped NCs.

Table 1 Photoluminescence lifetime values of Cd$_{1-x}$Zn$_x$Se$_{1-y}$S$_y$ NCs in different sample:

<table>
<thead>
<tr>
<th>Sample</th>
<th>$\tau_1$ (ns)</th>
<th>$A_1$ (%)</th>
<th>$\tau_2$ (ns)</th>
<th>$A_2$ (%)</th>
<th>$\tau_3$ (ns)</th>
<th>$A_3$ (%)</th>
<th>Adj. $R^2$ value</th>
<th>$\langle \tau \rangle$ (ns)</th>
<th>$\varnothing$</th>
<th>$1/\tau$ (ns$^{-1}$)</th>
<th>$1/t_{\varnothing}$ (ns$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>${\text{NC595}}_{\text{HDA}}$</td>
<td>46.8</td>
<td>35</td>
<td>20.6</td>
<td>51</td>
<td>6.8</td>
<td>14</td>
<td>0.999</td>
<td>27.83</td>
<td>0.52</td>
<td>0.0186</td>
<td>0.0172</td>
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<tr>
<td>${\text{NC597}}_{\text{OA}}$</td>
<td>51.2</td>
<td>20</td>
<td>10.3</td>
<td>30</td>
<td>2.35</td>
<td>50</td>
<td>0.998</td>
<td>14.4</td>
<td>0.26</td>
<td>0.01</td>
<td>0.051</td>
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<tr>
<td>${\text{NC596}}_{\text{TOPO}}$</td>
<td>21.3</td>
<td>23</td>
<td>7.2</td>
<td>44</td>
<td>1.9</td>
<td>33</td>
<td>0.999</td>
<td>8.7</td>
<td>0.16</td>
<td>0.01</td>
<td>0.096</td>
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</table>