Optoelectronic properties of dual emitting RNA mediated colloidal PbSe nanostructures

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Figure S1A The optical absorbance and fluorescence spectra of PbSe nanoparticles with Pb/Se molar ratio of 2 at pH: 8.5(a); 9.8 (b); 10.5(c); $\lambda_{ex} = 670$ nm.
Figure S1B Effect of molar ratio of Pb/Se: 1.0 (a); 2.0 (b); 3.0 (c) on the optical absorbance and fluorescence spectra of PbSe nanoparticles at pH 8.5 in the visible and NIR range.

Table S1A Effect of variation in [RNA] on depth of traps of RNA templated Q-PbSe in meV at 770 nm corresponding to different time constants at pH 8.5 and [Pb]/[Se]=2.

<table>
<thead>
<tr>
<th>Amount of RNA (g/100 ml)</th>
<th>$\tau_1$</th>
<th>$\tau_2$</th>
<th>$\tau_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.013</td>
<td>301.8</td>
<td>349.5</td>
<td>383.8</td>
</tr>
<tr>
<td>0.016</td>
<td>302.9</td>
<td>350.7</td>
<td>384.9</td>
</tr>
<tr>
<td>0.022 (RLS Fresh)</td>
<td>317.1</td>
<td>356.8</td>
<td>386.4</td>
</tr>
<tr>
<td>0.022 (RLS Aged)</td>
<td>274.3</td>
<td>343.0</td>
<td>378.0</td>
</tr>
<tr>
<td>0.025</td>
<td>305.1</td>
<td>357.7</td>
<td>386.5</td>
</tr>
</tbody>
</table>
**Table S1B** Effect of variation in [RNA] on depth of traps of RNA templated Q-PbSe in meV at 1000 nm at pH 8.5 and [Pb]/[Se]=2.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Depth of the Traps (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.019</td>
<td>317.7</td>
</tr>
<tr>
<td>0.022 (RLS Fresh)</td>
<td>319.3</td>
</tr>
<tr>
<td>0.022 (RLS Aged)</td>
<td>299.8</td>
</tr>
<tr>
<td>0.025</td>
<td>308.9</td>
</tr>
</tbody>
</table>

**Figure S2A** Effect of pH on fluorescence decay of RNA (0.022 g/100 ml) templated Q-PbSe ([Pb]/[Se]=2) in the visible region (λ<sub>ex</sub>=635 nm; λ<sub>fl</sub>=770nm).
**Figure S2B** Effect of pH: 8.5 (black); 9.8 (red); 10.5 (blue) on fluorescence decay of RNA (0.022 g/100 ml) templated Q-PbSe ([Pb]/[Se]) in the NIR region (λ<sub>ex</sub>=635 nm; λ<sub>em</sub>=1000 nm).

**Table S2A** Effect of pH on fluorescence lifetime of RNA (0.022 g/100 ml) templated Q-PbSe ([Pb]/[Se]=2) in the visible region (λ<sub>ex</sub>=635 nm; λ<sub>em</sub>=770 nm)

<table>
<thead>
<tr>
<th>pH</th>
<th>Component 1</th>
<th></th>
<th>Component 2</th>
<th></th>
<th>Component 3</th>
<th></th>
<th>&lt;τ&gt; (ns)</th>
<th>χ²</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.5</td>
<td>τ₁: 29.23</td>
<td>Emission%</td>
<td>τ₂: 140.75</td>
<td>Emission%</td>
<td>τ₃: 456.5</td>
<td>Emission%</td>
<td>320.0</td>
<td>1.21</td>
</tr>
<tr>
<td></td>
<td>(0.26)</td>
<td></td>
<td>(0.23)</td>
<td></td>
<td>(0.13)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9.8</td>
<td>τ₁: 14.31</td>
<td>Emission%</td>
<td>τ₂: 87.16</td>
<td>Emission%</td>
<td>τ₃: 308.2</td>
<td>Emission%</td>
<td>180.6</td>
<td>1.31</td>
</tr>
<tr>
<td></td>
<td>(0.23)</td>
<td></td>
<td>(0.23)</td>
<td></td>
<td>(0.06)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.5</td>
<td>τ₁: 7.2</td>
<td>Emission%</td>
<td>τ₂: 55.97</td>
<td>Emission%</td>
<td>τ₃: 212.7</td>
<td>Emission%</td>
<td>113.9</td>
<td>1.69</td>
</tr>
<tr>
<td></td>
<td>(0.28)</td>
<td></td>
<td>(0.26)</td>
<td></td>
<td>(0.05)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
(Value in bracket is pre-exponential factor corresponding to respective τ)

**Table S2A**’ Effect of pH on depth of traps of RNA (0.022 g/100 ml) templated Q-PbSe in meV at 770 nm corresponding to different time constants at pH 8.5 and [Pb]/[Se]=2.

<table>
<thead>
<tr>
<th>pH</th>
<th>τ₁</th>
<th>τ₂</th>
<th>τ₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.5</td>
<td>317.1</td>
<td>356.8</td>
<td>386.4</td>
</tr>
<tr>
<td>9.8</td>
<td>299.1</td>
<td>344.7</td>
<td>376.5</td>
</tr>
<tr>
<td>10.5</td>
<td>281.8</td>
<td>333.5</td>
<td>367.2</td>
</tr>
</tbody>
</table>

**Table S2B** Effect of variation in pH on fluorescence lifetime of RNA (0.022 g/100 ml) templated Q-PbSe in the NIR region at [Pb]/[Se]=2 (λₑₓ=635 nm; λₑₘ =1000 nm; Cut filter 830 nm).

<table>
<thead>
<tr>
<th>pH</th>
<th>τ (ns)</th>
<th>Emission%</th>
<th>χ²</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.5</td>
<td>31.8</td>
<td>100</td>
<td>1.0</td>
</tr>
<tr>
<td>9.8</td>
<td>23.61</td>
<td>100</td>
<td>1.02</td>
</tr>
<tr>
<td>10.5</td>
<td>23.98</td>
<td>100</td>
<td>1.0</td>
</tr>
</tbody>
</table>

**Table S2B’** Effect of variation in pH on depth of traps of RNA (0.022 g/100 ml) templated Q-PbSe in meV at 1000 nm and [Pb]/[Se]=2.

<table>
<thead>
<tr>
<th>pH</th>
<th>Depth of the Traps (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.5</td>
<td>319.3</td>
</tr>
<tr>
<td>9.8</td>
<td>312.2</td>
</tr>
<tr>
<td>10.5</td>
<td>311.8</td>
</tr>
</tbody>
</table>
**Figure S3A** Effect of variation in molar ratio of Pb/Se: 1.0 (a); 2.0 (b); 3.0 (c) on fluorescence decay of RNA (0.022 g/ 100 ml) templated Q-PbSe at pH=8.5 ($\lambda_{\text{ex}}$=635 nm; $\lambda_{\text{em}}$=770 nm).

**Figure S3B** Effect of variation in molar ratio of Pb/Se: 1 (a); 2(b); 3 (c) on fluorescence decay of RNA (0.022 g/ 100 ml) templated Q-PbSe at pH=8.5 ($\lambda_{\text{ex}}$=635 nm; $\lambda_{\text{em}}$=1000 nm).
Table S3A  Effect of variation in molar ratio of Pb/Se on fluorescence lifetime of RNA (0.022 g/100 ml) templated Q-PbSe at pH=8.5 ($\lambda_{ex}$=635 nm; $\lambda_{em}$=770 nm).

<table>
<thead>
<tr>
<th>[Pb]/[Se]</th>
<th>Component 1</th>
<th>Component 2</th>
<th>Component 3</th>
<th>$&lt;\tau&gt;$ (ns)</th>
<th>$\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\tau_1$</td>
<td>$\tau_2$</td>
<td>$\tau_3$</td>
<td>Emission%</td>
<td>Emission%</td>
</tr>
<tr>
<td>1</td>
<td>0.15 (297.5)</td>
<td>29.6 (0.18)</td>
<td>10.02</td>
<td>167.4 (2.34)</td>
<td>7.18</td>
</tr>
<tr>
<td>2</td>
<td>29.23 (0.26)</td>
<td>140.75 (0.23)</td>
<td>32.84</td>
<td>456.5 (0.13)</td>
<td>59.48</td>
</tr>
<tr>
<td>3</td>
<td>7.28 (0.24)</td>
<td>76.12 (0.23)</td>
<td>30.16</td>
<td>369.4 (0.10)</td>
<td>66.74</td>
</tr>
</tbody>
</table>

(Value in bracket is pre-exponential factor)

Table S3A’ Effect of variation in molar ratio of Pb/Se on depth of traps (in meV) of RNA (0.022 g/100 ml) templated Q-PbSe corresponding to different time constants at pH=8.5 in visible region at 770 nm.

<table>
<thead>
<tr>
<th>[Pb]/[Se]</th>
<th>$\tau_1$</th>
<th>$\tau_2$</th>
<th>$\tau_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>184.2</td>
<td>317.5</td>
<td>361.1</td>
</tr>
<tr>
<td>2</td>
<td>317.15</td>
<td>356.8</td>
<td>386.4</td>
</tr>
<tr>
<td>3</td>
<td>282.1</td>
<td>341.3</td>
<td>381.1</td>
</tr>
</tbody>
</table>
Table S3B Effect of molar ratio of Pb/Se on fluorescence lifetime of RNA (0.022 g/100 ml) templated Q-PbSe at pH=8.5 (λ_{ex}=635 nm; λ_{em}=1000 nm; Cut filter 830 nm).

<table>
<thead>
<tr>
<th>[Pb]/[Se]</th>
<th>Lifetime (ns)</th>
<th>Emission%</th>
<th>(\chi^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(&lt;\tau&gt;) (ns)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>20.04</td>
<td>100</td>
<td>1.04</td>
</tr>
<tr>
<td>2</td>
<td>31.8</td>
<td>100</td>
<td>1.0</td>
</tr>
<tr>
<td>3</td>
<td>23.96</td>
<td>100</td>
<td>1.01</td>
</tr>
</tbody>
</table>

Table S3B’ Effect of variation in molar ratio of Pb/Se on depth of traps (in meV) of RNA (0.022 g/100 ml) templated Q-PbSe at pH=8.5 in meV at 1000 nm.

<table>
<thead>
<tr>
<th>Molar Ratio Pb/Se</th>
<th>Depth of the Traps (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>307.6</td>
</tr>
<tr>
<td>2</td>
<td>319.3</td>
</tr>
<tr>
<td>3</td>
<td>312.1</td>
</tr>
</tbody>
</table>

Table S4A Effect of aging on the fluorescence lifetime of RLS (λ_{ex} = 635 nm; λ_{em} = 750 nm)

<table>
<thead>
<tr>
<th>Aged (in days)</th>
<th>Lifetime (ns)</th>
<th>&lt;\tau&gt; (ns)</th>
<th>(\chi^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Component 1</td>
<td>Component 2</td>
<td>Component 3</td>
</tr>
<tr>
<td></td>
<td>(\tau_1)</td>
<td>Emission%</td>
<td>(\tau_2)</td>
</tr>
<tr>
<td>0</td>
<td>15.8 (0.42)</td>
<td>9.54</td>
<td>107.8 (0.26)</td>
</tr>
<tr>
<td>15</td>
<td>9.2 (0.34)</td>
<td>4.44</td>
<td>84.8 (0.26)</td>
</tr>
<tr>
<td>30</td>
<td>1.2 (17.2)</td>
<td>3.64</td>
<td>52.5 (3.25)</td>
</tr>
</tbody>
</table>

(Value in bracket is pre-exponential factor corresponding to respective \(\tau\))
**Table S4A** Effect of aging on depth of traps (in meV) of RLS corresponding to different time constants at 750 nm ($\lambda_{ex} = 635$ nm; $\lambda_{em} = 750$ nm)

<table>
<thead>
<tr>
<th>Aged (in days)</th>
<th>$\tau_1$</th>
<th>$\tau_2$</th>
<th>$\tau_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>301.6</td>
<td>350.0</td>
<td>386.6</td>
</tr>
<tr>
<td>15</td>
<td>288.0</td>
<td>344.0</td>
<td>380.4</td>
</tr>
<tr>
<td>30</td>
<td>234.8</td>
<td>331.9</td>
<td>375.9</td>
</tr>
</tbody>
</table>

**Table S4B** Effect of aging on depth of traps (in meV) of RLS corresponding to time constant at 1000 nm ($\lambda_{ex} = 635$ nm).

<table>
<thead>
<tr>
<th>Aged (in days)</th>
<th>Depth of the Traps (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>319.3</td>
</tr>
<tr>
<td>30</td>
<td>299.3</td>
</tr>
</tbody>
</table>

**Table S5**: XPS spectral data of RLS

<table>
<thead>
<tr>
<th>Sample</th>
<th>Peaks/orbital</th>
<th>B.E.(eV) Literature in reference to PbSe</th>
<th>B.E.(eV) Observed</th>
</tr>
</thead>
<tbody>
<tr>
<td>PbSe</td>
<td>Pb 4f$_{7/2}$</td>
<td>142.5</td>
<td>141.2</td>
</tr>
<tr>
<td></td>
<td>Pb 4f$_{5/2}$</td>
<td>137.3</td>
<td>136.2</td>
</tr>
<tr>
<td>PbSe</td>
<td>Se 3d$_{5/2}$</td>
<td>53.3</td>
<td>53.6</td>
</tr>
<tr>
<td></td>
<td>Se 3d$_{3/2}$</td>
<td>54.18</td>
<td>54.5</td>
</tr>
<tr>
<td>Pb(OH)$_2$</td>
<td>O1s</td>
<td>530.8</td>
<td>528.7 and 529.8 ($\text{Pb(OH)}_2$ and Hydrated Pb$^{2+}$ in PbSe)</td>
</tr>
</tbody>
</table>
Table S6 CD spectral data of RNA (R), RNA-Pb\(^{2+}\) (RL) and RLS

<table>
<thead>
<tr>
<th>Sample</th>
<th>Peak 1</th>
<th>Peak 2</th>
<th>Peak 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>RNA (R)</td>
<td>X = 207.6, Y = -2.6</td>
<td>X = 242.9, Y = -2.19</td>
<td>X = 271.49, Y = 7.79</td>
</tr>
<tr>
<td>RNA-Pb(^{2+}) (RL)</td>
<td>X = 208.5, Y = -1.8</td>
<td>X = 240.8, Y = -1.6</td>
<td>X = 274.8, Y = 4.2</td>
</tr>
<tr>
<td>RLS Fresh</td>
<td>X = 208.9, Y = -1.9</td>
<td>X = 242.9, Y = -2.1</td>
<td>X = 272.7, Y = 4.44</td>
</tr>
<tr>
<td>RLS Aged</td>
<td>X = 212.2, Y = 0.37</td>
<td>X = 236.2, Y = -0.8</td>
<td>X = 272.2, Y = 2.9</td>
</tr>
</tbody>
</table>

Table S7 Effect of [RNA] on surface roughness and average maximum surface roughness of RNA templated PbSe at pH 8.5 and [Pb]/[Se]=2.

<table>
<thead>
<tr>
<th>[RNA] (g/100 ml)</th>
<th>Surface Roughness (nm)</th>
<th>Average Maximum Surface Roughness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.019</td>
<td>4.0-23.0</td>
<td>14</td>
</tr>
<tr>
<td>0.022</td>
<td>0.8-3.5</td>
<td>1.7</td>
</tr>
<tr>
<td>0.025</td>
<td>5.0-25.0</td>
<td>15.5</td>
</tr>
</tbody>
</table>
Table S8 Effect of pH on surface roughness and average maximum surface roughness of RNA (0.022 g/100 ml) templated PbSe at [Pb]/[Se]=2.

<table>
<thead>
<tr>
<th>pH</th>
<th>Surface Roughness (nm)</th>
<th>Average Maximum Surface Roughness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.5</td>
<td>0.8-3.5</td>
<td>1.7</td>
</tr>
<tr>
<td>10.5</td>
<td>2.8-8.4</td>
<td>5.7</td>
</tr>
</tbody>
</table>

Table S9 Effect of [Pb]/[Se] on surface roughness and average maximum surface roughness of RNA(0.022 g/100 ml) templated PbSe at pH 8.5.

<table>
<thead>
<tr>
<th>[Pb]/[Se]</th>
<th>Surface Roughness (nm)</th>
<th>Average Maximum Surface Roughness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0-10.2</td>
<td>5.0</td>
</tr>
<tr>
<td>2</td>
<td>0.8-3.5</td>
<td>1.7</td>
</tr>
<tr>
<td>3</td>
<td>2.0-15.0</td>
<td>8.2</td>
</tr>
</tbody>
</table>