Critical Assessment of Wet-chemical Oxidation Synthesis of Silicon Quantum Dots

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1. Elemental analysis of Si QDs and Control

Table S1. Elemental composition of Si QDs and Control.

<table>
<thead>
<tr>
<th></th>
<th>Bromine (%)</th>
<th>Carbon (%)</th>
<th>Silicon (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si QDs (18 h)</td>
<td>6.5</td>
<td>61.2</td>
<td>2.1</td>
</tr>
<tr>
<td>Si QDs (60 h)</td>
<td>3.9</td>
<td>64.3</td>
<td>2.2</td>
</tr>
<tr>
<td>Control</td>
<td>11.2</td>
<td>69.7</td>
<td>0.4</td>
</tr>
</tbody>
</table>

2. XPS data Si QDs and Control

Figure S1. Wide-scan spectrum XPS of Si QDs.

Figure S2. Deconvoluted C 1s (a), O 1s (b), and Si 2p (c) XPS spectra for Si QDs.
Figure S3. Wide-scan spectrum XPS of Control.

Figure S4. Deconvoluted C 1s (a), O 1s (b), and Si 2p (c) XPS spectra for the Control.
3. Comparison between Si QDs for 18 h and 60 h reaction duration

![Graphs showing absorbance and emission of Si QDs for 18 and 60 h reaction duration](image)

**Figure S5.** Absorbance (a) and emission of Si QDs (18 and 60 h), and the Control for excitation at 300 (b), 350 (c) and 400 nm (d), respectively.

4. Quantum yield calculation

Quantum yield can be calculated by applying Equation 1.¹

\[
Q = Q_R \times \frac{I}{I_R} \times \frac{OD}{OD_R} \times \frac{n^2}{n^2_R}
\] ¹

Q is the quantum yield, I the integrated fluorescence intensity, OD the optical density (i.e. absorbance), and n the refractive index. The subscript R refers to the reference. For quantum yield determination, 9,10-diphenylanthracene (9,10-DPA) in ethanol was chosen as reference, with a quantum yield of approximately 95%.²
5. Full SEC traces with absorbance and fluorescence of Si QDs and Control

![Graphs showing absorbance and fluorescence traces for Si QDs and Control](image)

**Figure S6.** Full SEC trace of Si QDs with absorbance (a) and fluorescence (b), and trace of Control with absorbance (c) and fluorescence (d).

6. Absorbance SEC traces of Si QDs and Control

![Graph showing absorbance traces for Si QDs and Control](image)

**Figure S7.** SEC trace with absorbance of Si QDs (a) and the Control (b) at wavelengths from 250-450 nm.
7. $^1$H NMR spectroscopy of brominated n-octane

![NMR Spectroscopy Image]

**Figure S8.** $^1$H NMR spectroscopy upon bromination of n-octane in chloroform-d.

Integration of peaks denoted with (*) and (=,o) do not match entirely, due to baseline drifting caused by a high n-octane concentration. As a result, integrations of the latter peaks were overestimated.

**References**