**Supplementary information**

Highly luminescent and cytocompatible cationic Ag$_2$S NIR-emitting quantum dots for gene transfection and optical imaging

Fatma Demir Duman, Ibrahim Hocaoglu, Deniz Gulzem Ozurk, Alper Kiraz, Devrim Gozuacik, Havva Yagci Acar *

Quantum Yield Calculation

![Plot of integrated luminescence intensities](image1)

![Plot of absorbance](image2)

Fig. S1. Photoluminescence spectra of aqueous Ag$_2$S NIRQDs (80/20 PEI/2MPA at pH 7.4 in water (left) and LDS 798 NIR dye in MeOH (right) at different concentrations.

![Plot of integrated fluorescence intensity vs. absorbance](image3)

![Equation table](table)

Fig. S2. Plot of the integrated luminescence intensities of the dye and QD samples against the absorbance. Inset shows the slope of each line.

**Influence of Ag/S mole ratio on particle properties**

In the synthesis of PEI coated Ag$_2$S NIRQDs, Ag/S mole ratio of 2.5 and 4 were studied under identical conditions: Coating/Ag ratio of 5, pH 10. Photoluminescence and absorbance graphs of these two particles prepared at room temperature and quenched in 75 min were shown in Fig. S3.
Influence of reaction time on particle properties
Aliquots from reaction mixture were taken out with a syringe at different time points and particle growth and luminescence peak were monitored by UV-absorbance and photoluminescence spectra (Fig. S5). Table S1 summarizes the effects of reaction time on the particle properties for Ag$_2$S NIRQDs synthesized with 60/40 PEI/2MPA at pH 10 with Ag/S ratio of 4 and coating/Ag ratio of 5 at room temperature.

Influence of Ag/PEI ratio on particle properties
In order to determine the best Ag/PEI ratio which would provide effective surface passivization and strong luminescence as well as to influence the crystal size, different Ag/PEI ratios were studied under identical reaction conditions: Ag/S=4, room temperature, pH 10. Photoluminescence and absorbance graphs of PEI coated Ag$_2$S NIRQDs synthesized with Ag/PEI ratio of 1/5 and 1/15 are shown in Fig. S4.

Fig. S3. Photoluminescence (a) and absorbance (b) spectra of PEI coated Ag$_2$S QD prepared at different Ag/S mole ratios.

Fig. S4. Photoluminescence (a) and absorbance (b) spectra of PEI coated Ag$_2$S NIRQDs prepared at different Ag/PEI mole ratios.

Fig. S5. (a) Absorbance calibrated photoluminescence and (b) Normalized absorbance graphs of the Ag$_2$S NIRQDs prepared with PEI/2MPA 60/40 mixed coating at different time points during the reaction.
Table S1. Effect of the reaction time on the properties of Ag$_2$S NIRQDs.

<table>
<thead>
<tr>
<th>Reaction time (min)</th>
<th>$\lambda_{\text{abs}(\text{cutoff})}$ (nm)</th>
<th>Size (nm)</th>
<th>Band gap (eV)</th>
<th>$\lambda_{\text{em}}$(max) (nm)</th>
<th>FWHM (nm)</th>
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<tbody>
<tr>
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<td>1.60</td>
<td>820</td>
<td>147</td>
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<tr>
<td>20</td>
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<td>2.52</td>
<td>1.60</td>
<td>825</td>
<td>148</td>
</tr>
<tr>
<td>35</td>
<td>777</td>
<td>2.52</td>
<td>1.60</td>
<td>828</td>
<td>152</td>
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<td>1.60</td>
<td>828</td>
<td>148</td>
</tr>
</tbody>
</table>

$^a)$ Absorbance onset; $^b)$ Diameter of Ag$_2$S crystal calculated by Brus equation. Reaction formulation and conditions: Ag/S = 4, Ag/PEI = 1 : 3, Ag/2MPA = 1 : 2, reaction pH : 10, Room Temperature.

Effect of PEI/2MPA ratio on particle properties

Fig. S6 is the normalized absorbance spectra of the quantum dots prepared with PEI/2MPA coating under identical conditions.

![Normalized absorbance spectra of Ag$_2$S NIRQDs prepared with different PEI/2MPA ratios (Ag : S = 4, RT, reaction pH : 10, 5 min reaction).](image)

Fig. S6. Absorbance spectra of Ag$_2$S NIRQDs prepared with different PEI/2MPA ratios (Ag : S = 4, RT, reaction pH : 10, 5 min reaction).

Influence of reaction pH on particle properties

Ag$_2$S NIRQDs synthesized with PEI/2MPA mixture at 60/40 and 80/20 ratios were prepared at different pH values. Fig. S7 shows the normalized absorbance graphs of these synthesized Ag$_2$S NIRQDs.

![Normalized absorbance graphs of Ag$_2$S NIRQDs synthesized in different pH values: (a) 60 % PEI/40 % 2MPA; (b) 80 % PEI/20 % 2MPA.](image)

Fig. S7. Normalized absorbance graphs of the PEI/2MPA coated Ag$_2$S NIRQDs synthesized in different pH values: (a) 60 % PEI / 40 % 2MPA; (b) 80 % PEI / 20 % 2MPA.
**pH dependent luminescence behavior of Ag\textsubscript{2}S NIRQDs**

pH of the aqueous Ag\textsubscript{2}S NIRQDs synthesized at pH 9 with PEI/2MPA mole ratio of 80/20 were adjusted to basic (pH 9.0), neutral (pH 7.4) and acidic (pH 5.5) pH, after being washed. Fig. S8 shows the normalized absorbance spectra of these QDs.

![Normalized absorbance graphes of Ag\textsubscript{2}S NIRQDs (80/20 PEI/2MPA) at different pH values.](image1)

**Fig. S8.** Normalized absorbance graphes of Ag\textsubscript{2}S NIRQDs (80/20 PEI/2MPA) at different pH values.

**Long term stability of Ag\textsubscript{2}S-PEI/2MPA QDs**

![Normalized absorbance spectra of Ag\textsubscript{2}S NIRQDs with 80/20 PEI/2MPA at different time points following its synthesis.](image2)

**Fig. S9.** Normalized absorbance spectra of Ag\textsubscript{2}S NIRQDs with 80/20 PEI/2MPA at different time points following its synthesis.

**XRD analysis of Ag\textsubscript{2}S NIRQDs**

![XRD analysis of Ag\textsubscript{2}S NIRQDs](image3)
Fig. S10. XRD pattern of the Ag$_2$S NiRQD.

**Optical Imaging of HeLa cells**

Near IR images of Ag$_2$S NiRQD untreated and treated cells were recorded on a CLM. The red color shows quantum dots in the cell. The scale means the intensity of QD emission.

![Confocal images of HeLa cells](image)

Fig. S11. Confocal images of HeLa cells. Cells untreated with QDs (a), cells with QDs (b). Red color shows the quantum dots.