Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary information

Highly luminescent and cytocompatible cationic Ag_2S NIR-emitting quantum dots for gene transfection and optical imaging

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Quantum Yield Calculation

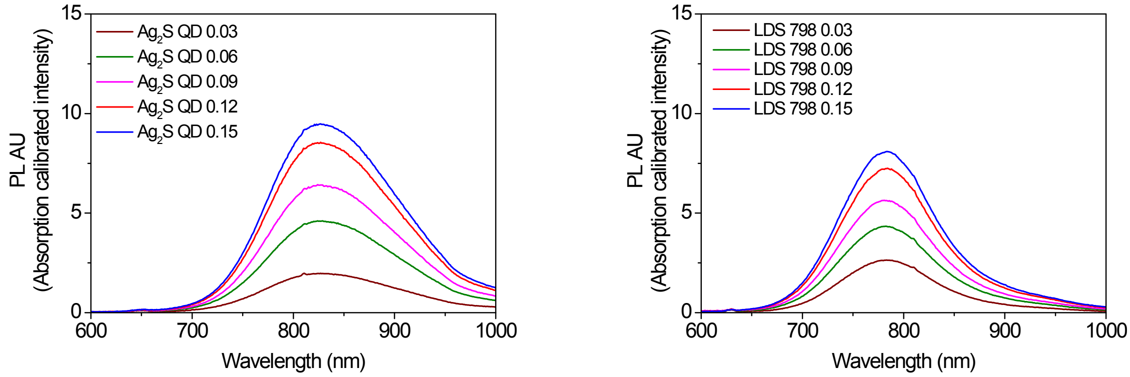

Fig. S1. Photoluminescence spectra of aqueous Ag_2S NIRQDs (80/20 PEI/2MPA at pH7.4 in water (left) and LDS 798 NIR dye in MeOH (right) at different concentrations.

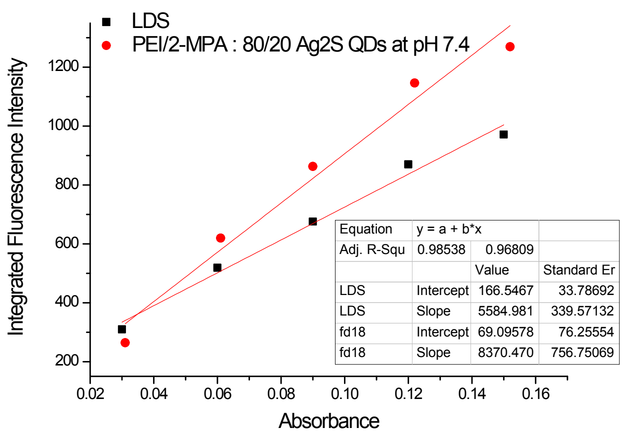

Fig. S2. Plot of the the integrated luminesence intensities of the dye and QD samples against the absorbance. Inset shows the slope of each line.

Influence of Ag/S mole ratio on particle properties

In the synthesis of PEI coated Ag_2S NIRQDs, Ag/S mole ratio of 2.5 and 4 were studied under identical conditions: Coating/Ag ratio of 5, pH 10. Photoluminesence and absorbance graphs of these two particles prepared at room temperature and quenched in 75 min were shown in Fig. S3.

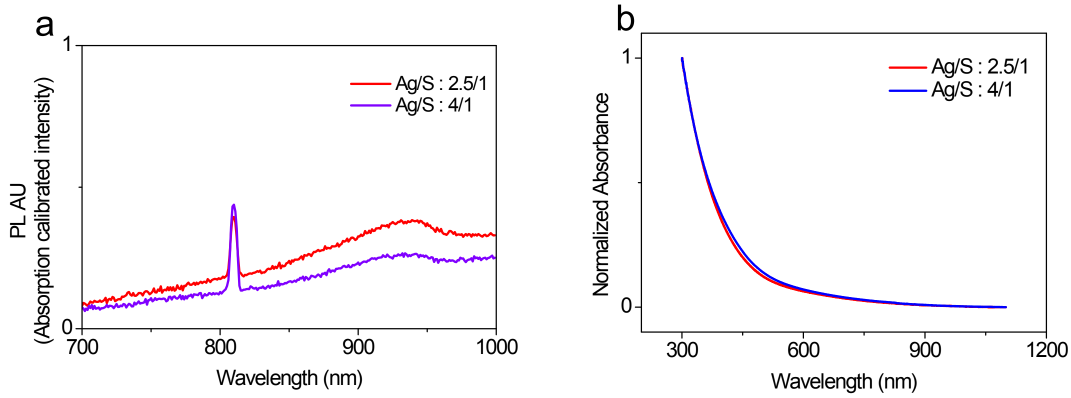

Fig. S3. Photoluminescence (a) and absorbance (b) spectra of PEI coated Ag_2S QD prepared at different Ag/S mole ratios.

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_2S NIRQDs synthesized with Ag/PEI ratio of 1/5 and 1/15 are shown in Fig. S4.

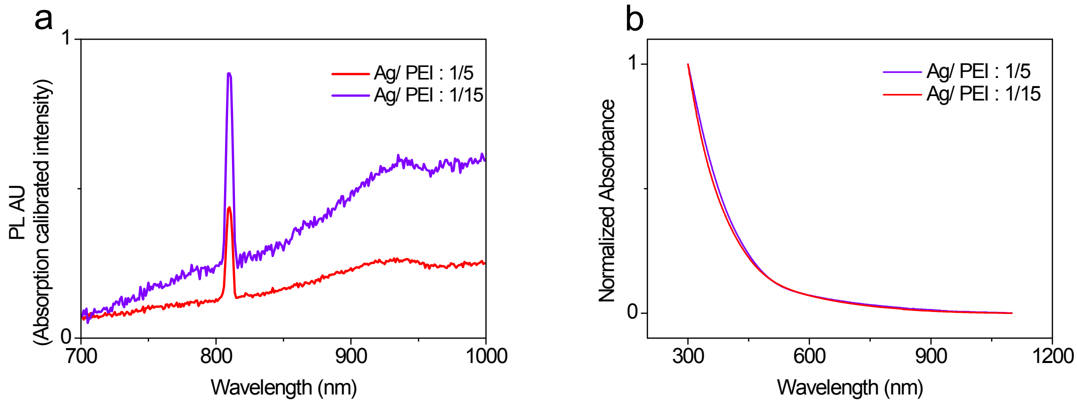

Fig. S4. Photoluminescence (a) and absorbance (b) spectra of PEI coated Ag_2S NIRQDs prepared at different Ag/PEI mole ratios.

Influence of reaction tine 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_2S 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.

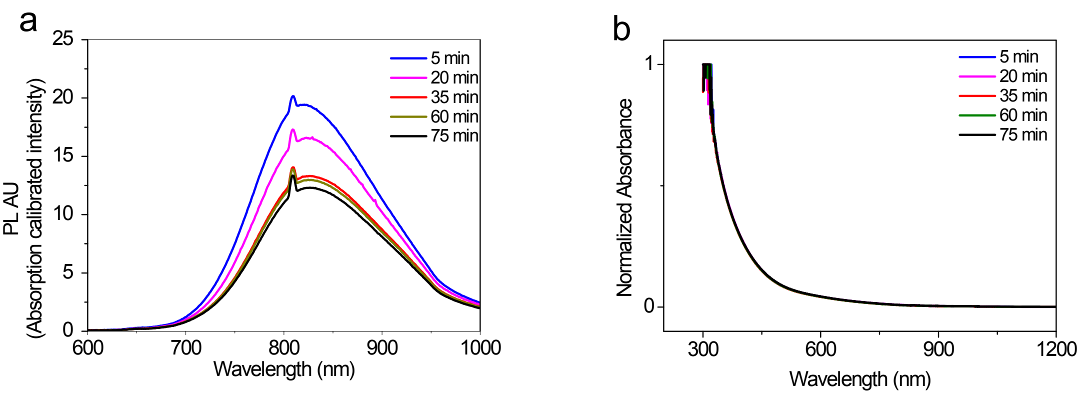

Fig. S5. (a) Absorbance calibrated photoluminescence and (b) Normalized absorbance graphs of the Ag_2S NIRQDs prepared with PEI/2MPA 60/40 mixed coating at different time points during the reaction.

Table S1. Effect of the reaction time on the properties of Ag_2S NIRQDs.

Reaction time (min)	$\lambda_{abs(cutoff)}$[a] (nm)	Size[b] (nm)	Band gap (eV)	$\lambda_{em\,(max)}$ (nm)	FWHM (nm)
5	777	2.52	1.60	820	147
20	777	2.52	1.60	825	148
35	777	2.52	1.60	828	152
60	777	2.52	1.60	828	150
75	777	2.52	1.60	828	148

[a] Absorbance onset; [b] Diameter of Ag_2S 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.

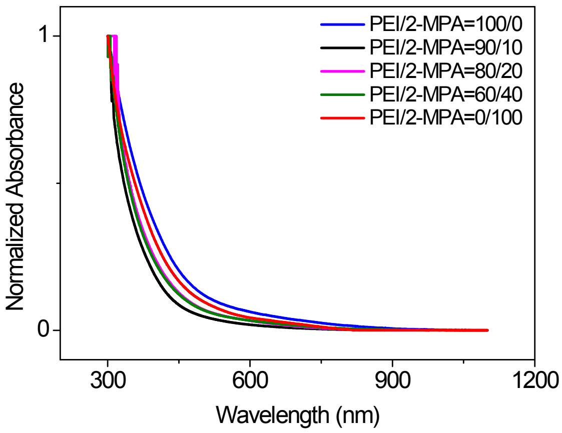

Fig. S6. Absorbance spectra of Ag_2S NIRQDs prepared with different PEI/ 2MPA ratios (Ag : S = 4, RT, reaction pH : 10, 5 min reaction).

Influence of reaction pH on particle properties

Ag_2S 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_2S NIRQDs.

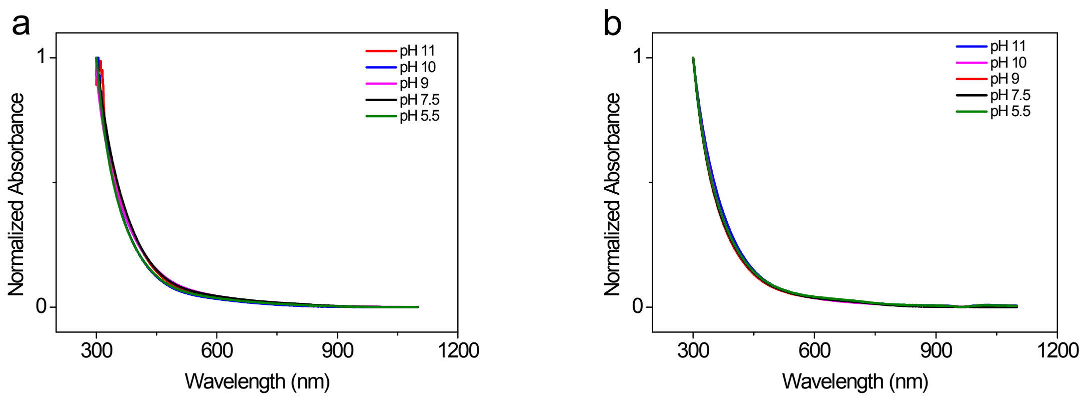

Fig. S7. Normalized absorbance graphs of the PEI/2MPA coated Ag_2S NIRQDs synthesized in different pH values: (a) 60 % PEI / 40 % 2MPA ; (b) 80 % PEI / 20 % 2MPA.

pH dependent luminesence behavior of Ag_2S NIRQDs

pH of the aqueous Ag_2S 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.

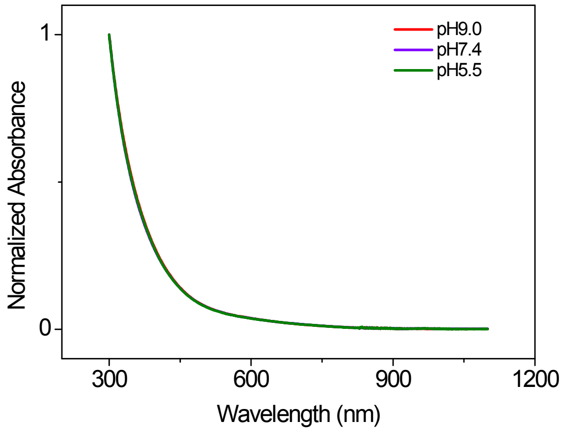

Fig. S8. Normalized absorbance graphes of Ag_2S NIRQDs (80/20 PEI/2MPA) at different pH values.

Long term stability of Ag_2S-PEI/2MPA QDs

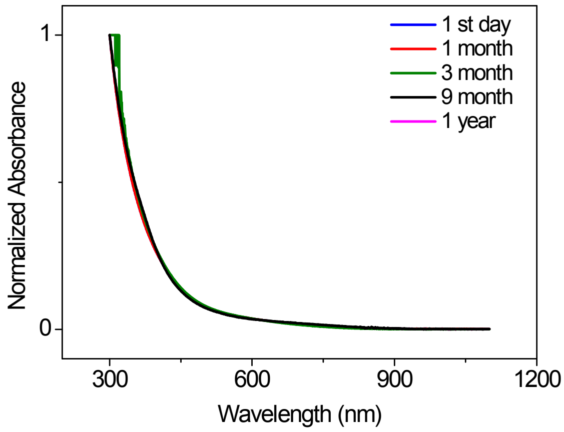

Fig. S9. Normalized absorbance spectra of Ag_2S NIRQDs with 80/20 PEI/2MPA at different time points following its synthesis.

XRD analysis of Ag_2S NIRQDs

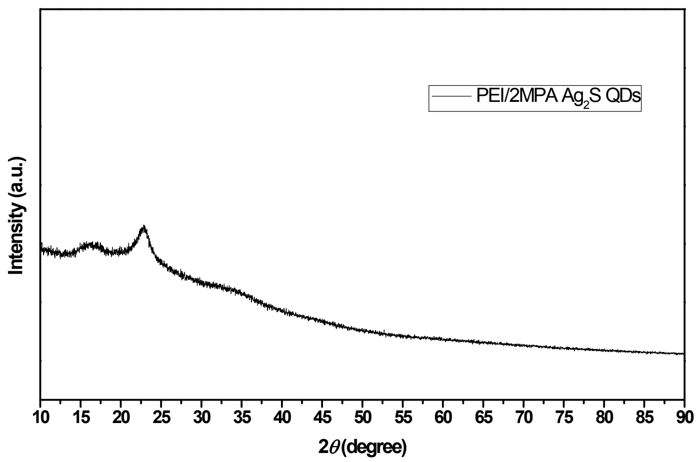

Fig. S10. XRD pattern of the Ag_2S NIRQD.

Optical Imaging of HeLa cells

Near IR images of Ag_2S 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.

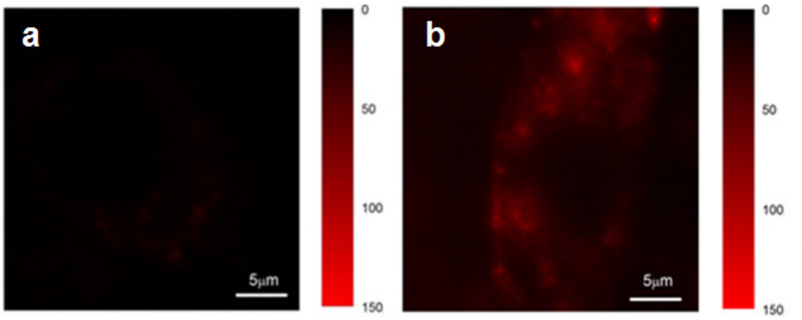

Fig. S11. Confocal images of HeLa cells. Cells untreated with QDs (a), cells with QDs (b). Red color shows the quantum dots.