Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information for:

The Influence of Surface Passivation on Electronic Energy Relaxation of CdSe and CdSe/CdS Nanocrystals Studied Using Visible and Near Infrared Transient Absorption Spectroscopy

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The uniqueness of the four exponential global fitting components of CdSe QDs were investigated by examining the reduced χ^2 error surfaces of the independent parameters extracted from convergent fits based on a wide range of initial values. Each principle kinetic was fitted though fixing one time constant in a reasonable range and allowing the other time constants to adjust. The fitting was repeated again by changing the value of fixed time constants. The fitting results obtained from the best fits for each sample are summarized in Tables S1-S5.

1. 400-nm photon excitation

Table S1. Amplitudes and time constants obtained from ground state bleach fitting of different CdSe nanocrystal sizes.

	CdSe-2.34 eV	CdSe-2.24 eV	CdSe-2.17 eV	CdSe-2.10 eV
A_1	-0.317±0.004	-0.183±0.008	-0.151±0.02	-0.124±0.01
A_2	-0.243±0.003	-0.238±0.008	-0.132±0.02	-0.137±0.007
A_3	-0.440±0.002	-0.579±0.002	-0.716±0.007	-0.739±0.009
t_1(ps)	7.23±0.16	9.261±0.50	23.2±0.48	66.4±4.80
t_2(ps)	73.5±2.6	51.945±2.5	143±30.6	402±64.0
t_3(ps)	5980±111	7884.683±118	8911±423	6492±225

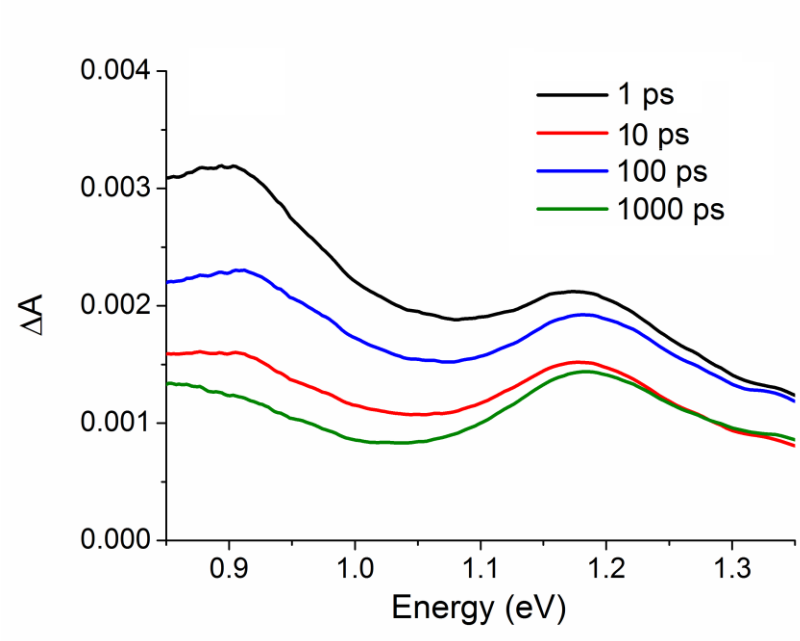

Figure S1. NIR transient absorption spectra of CdSe at several different pump-probe delay time after 400 nm excitation (800nJ).

Table S2. Time constants obtained from global analysis of CdSe QDs NIR TA spectra.

	CdSe-2.34 eV	CdSe-2.24 eV	CdSe-2.17 eV	CdSe-2.10 eV
t_1(ps)	2.12±0.208	4.07±1.02	4.65±0.177	3.92±0.279
t_2(ps)	13.9±0.271	31.53±1.51	28.7±1.16	29.7±14.7
t_3(ps)	128±40.2	299±28.8	179±25.5	199±46.8
t_4(ps)	6749±527	6618±1594	9094±1153	6067±785

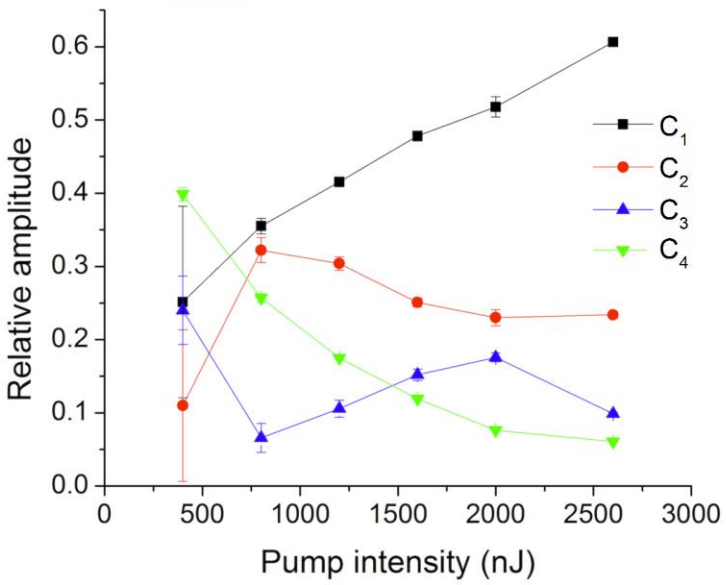

Figure S2. Excitation energy dependence of relative amplitudes of components extracted from global analysis.

Table S3. Time constants and amplitude coefficients obtained from global analysis of CdSe/CdS NIR TA spectra.

	1ML	3ML	5ML
A_1	0.205±0.06	0.363±0.025	0.400±0.087
A_2	0.327±0.029	0.381±0.028	0.413±0.037
A_3	0.468±0.032	0.257±0.017	0.187±0.056
t_1(ps)	6.83±0.772	8.73±1.71	6.50±0.58
t_2(ps)	80.9±0.794	96.3±8.24	72.8±2.91
t_3(ps)	8876±423	49219±869	1973±453

2. 530-nm photon excitation.

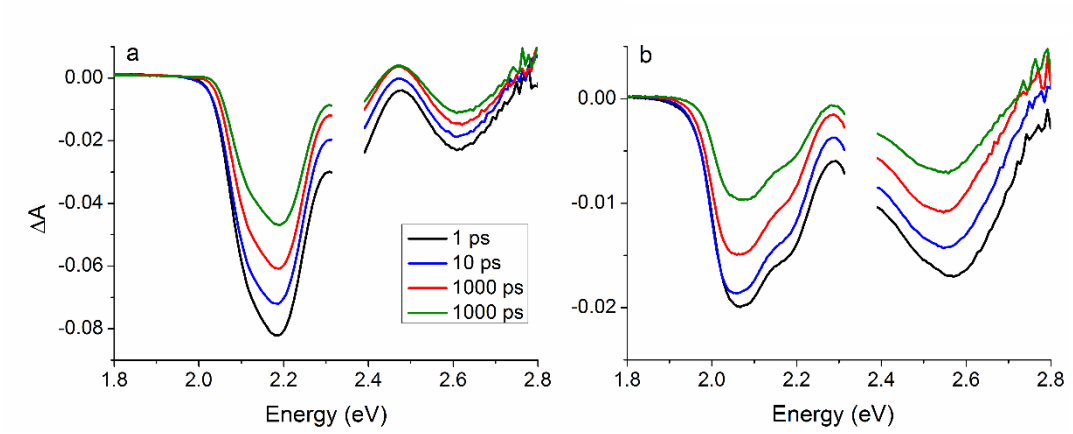

Figure S3. Visible transient absorption spectra of (a) CdSe and (b) CdSe/CdS-3ML NCs at different pump-probe delay time after 530 nm excitation (500nJ).

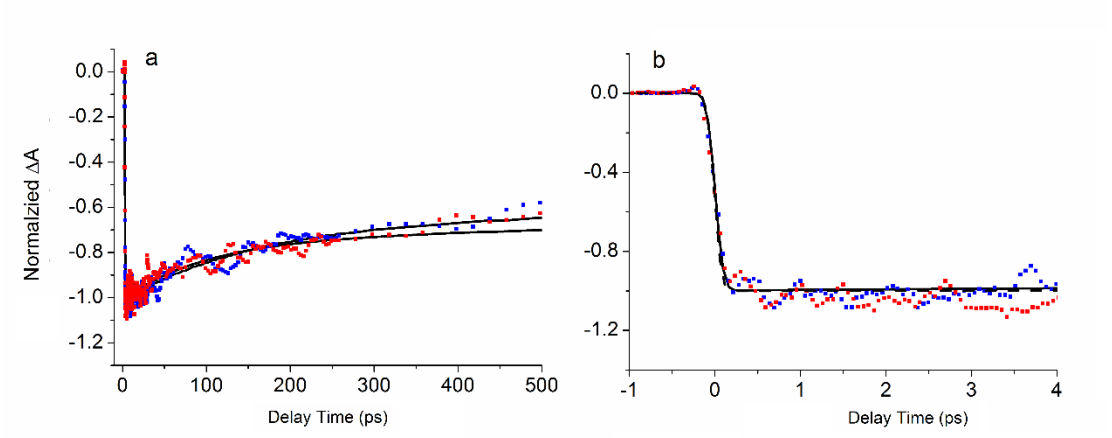

Figure S4. Bleach recovery kinetics of CdSe (blue) and CdSe/CdS-3ML (red) NCs at different under 530 nm excitation (500nJ).

Table S4. Amplitudes and time constants obtained from ground state bleach fitting of CdSe core and CdSe/CdS core/shell QDs.

	CdSe core	CdSe/CdS-3ML
A_1	-0.257±0.032	-0.344±0.012
A_2	-0.743±0.032	-0.656±0.012
t_1(ps)	82.3±15.4	160±21.1
t_2(ps)	6883±1321	7750±553

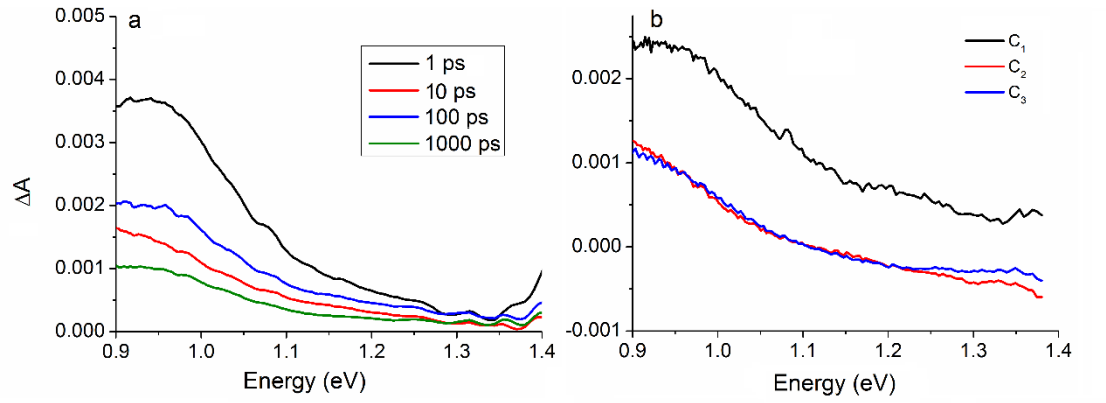

Figure S5. (a) NIR transient absorption spectra of CdSe/CdS-3ML NCs at different pump-probe delay time after 530 nm excitation (500nJ). (b) Decomposition of the NIR transient absorption spectra of the CdSe/CdS-3ML under 530nm excitation.

Table S5. Time constants and amplitude coefficients obtained from global analysis of CdSe/CdS-3ML NIR TA spectra under 530 nm excitation.

3ML			
A_1	0.497±0.057	t_1(ps)	2.54±0.48
A_2	0.245±0.037	t_2(ps)	69.7±9.84
A_3	0.258±0.031	t_3(ns)	14.5±4.8