Supporting Information: Thin CdSe shell boosts the electron transfer from CdTe quantum dots to methylene blue

L. Dworak,^a S. Roth,^a M. P. Scheffer,^b A. Frangakis^b and J. Wachtveitl^a⁺

^a Institute of Physical and Theoretical Chemistry, Goethe–University Frankfurt, Max-von-Laue-Str. 7, D–60438 Frankfurt am Main.

^b·Buchmann Institute for Molecular Life Sciences, Goethe-University Frankfurt, Max-von-Laue-Str. 15, D-60438 Frankfurt am Main.

†Tel.: +49 (0)69 798 29351, E-mail: wveitl@theochem.uni-frankfurt.de



Figure S1. (a) Coherent artefact measured in

toluene at a probe wavelength of 590 nm and fit of the data. The fit yielded a cross correlation width of the setup of 110 fs which corresponds to the time resolution. (b) Spectrum of the excitation pulse applied in the TA measurements. The spectrum was recorded with an Ocean Optics S2000 multi-channel fiber optic spectrometer system.

2 TRANSMISSION ELECTRON MICROSCOPY



Figure S2. Class averages of (a) CdTe and (b) CdTe/CdSe nanocrystals. Each picture represents an average of ~250 particles. The boxes consist of 128×128 pixels with a pixel size of 0.99 Å.



3.1 Determination of the MB extinction coefficient

Figure S3. (left) Calibration curve for the determination of the extinction coefficient of MB adsorbed on the surface of CdTe QD. Absorption spectra were recorded in cuvettes of 4 mm optical path length. Linear fit analysis yielded an extinction coefficient of 3.66×10^4 M⁻¹ cm⁻¹. (right) Stern–Volmer-type plots representing the quenching effect of MB on CdTe QD PL intensity. For the experiments, the QD concentration is 5.8×10^{-6} M. The nonlinear behavior indicates a mixed contribution from dynamic and static fluorescence quenching mechanism.



3.2 Determination of the methylene blue absorption at the surfaces of different QD

Figure S4. Absorption spectra of (a) CdTe QD, (b) CdTe/CdSe QD and the corresponding complexes. Methylene blue spectra were obtained from the differences of the MB-QD and QD spectra.



4.1 Pump-power dependent measurements

Figure S5. (a) Single transient traces recorded after excitation of CdTe QD at 490 nm with different pump pulse energies. (b) Normalized transient traces; at energies <14 nJ the exciton dynamics exhibit no dependence on the pump pulse energy indicative of the single exciton regime.

4.2 MB-CdTe QD complexes



Figure S6. Spectra at fixed delay times recorded for (a) MB:CdTe QD 0.6:1 and (b) MB:CdTe QD 2.2:1 complexes after excitation of the QD at 490 nm.

4.3 MB-CdTe/CdSe QD complexes



Figure S7. Spectra at fixed delay times recorded for (a) MB:CdTe/CdSe QD 0.7:1 and (b) MB:CdTe/CdSe QD 2.1:1 complexes after excitation of the QD at 490 nm.