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Supporting Information for "The Curious Case of CdTe/CdS: Photoabsorption versus Photoemission"

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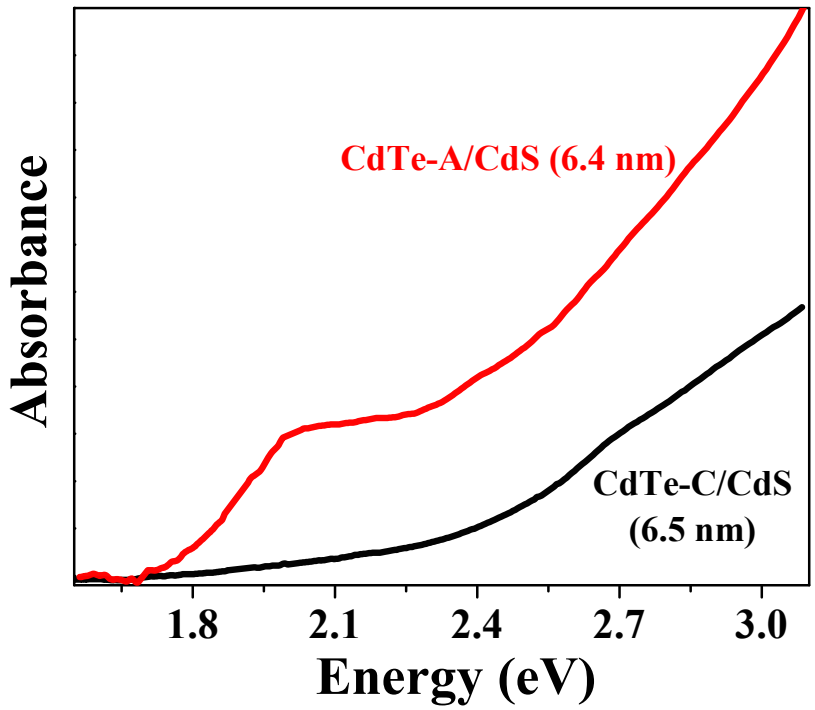

Figure S1. Absorption features of similar size CdTe-C/CdS (black line) and CdTe-A/CdS (red line) nanoparticles.

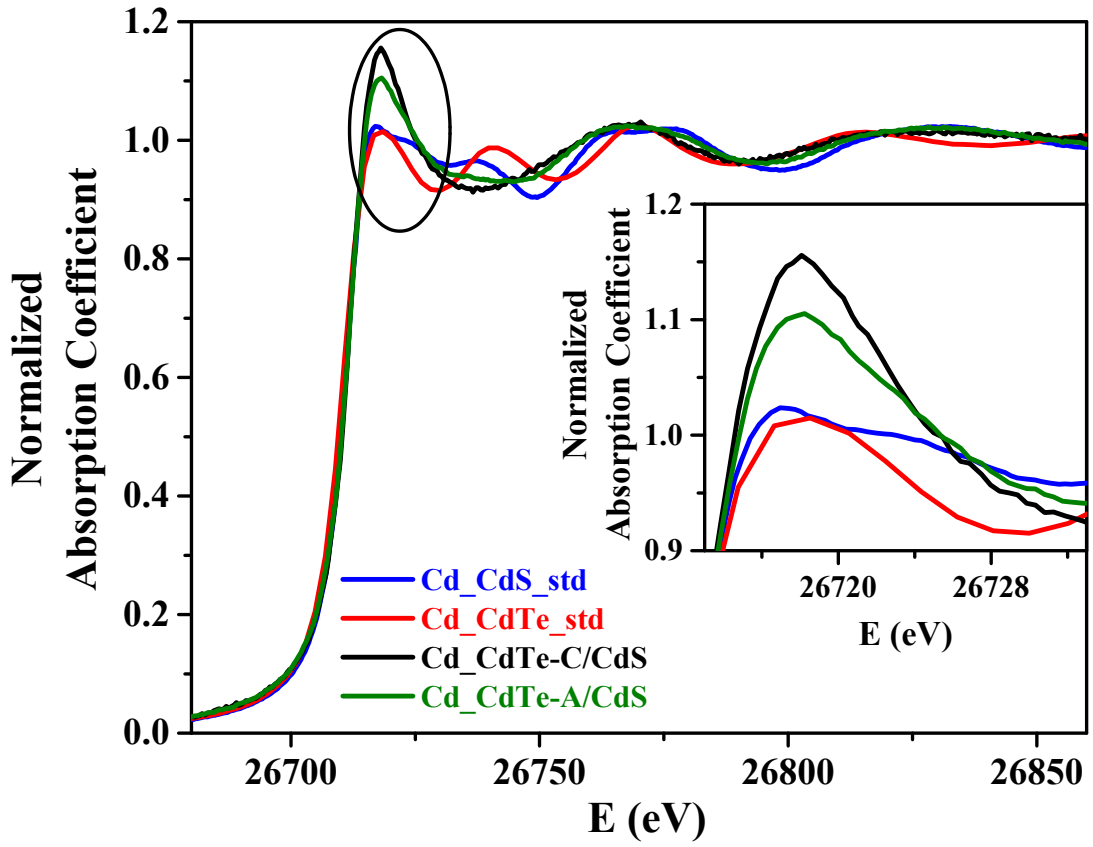

Figure S2. Cd edge X-ray Absorption Near Edge Structure (XANES) of both CdTe/CdS core/shell and alloy quantum dots.

The white line for the Cd edge of the alloy sample and core shell sample is higher than the Cd edge of CdS and CdTe standard samples because in both these samples, Cd atoms are slightly oxidized as some of the Cd atoms are on the surface. However, the number of Cd atoms which are oxidized is very few and no Cd-O bond was needed to fit Cd edge in both the samples.

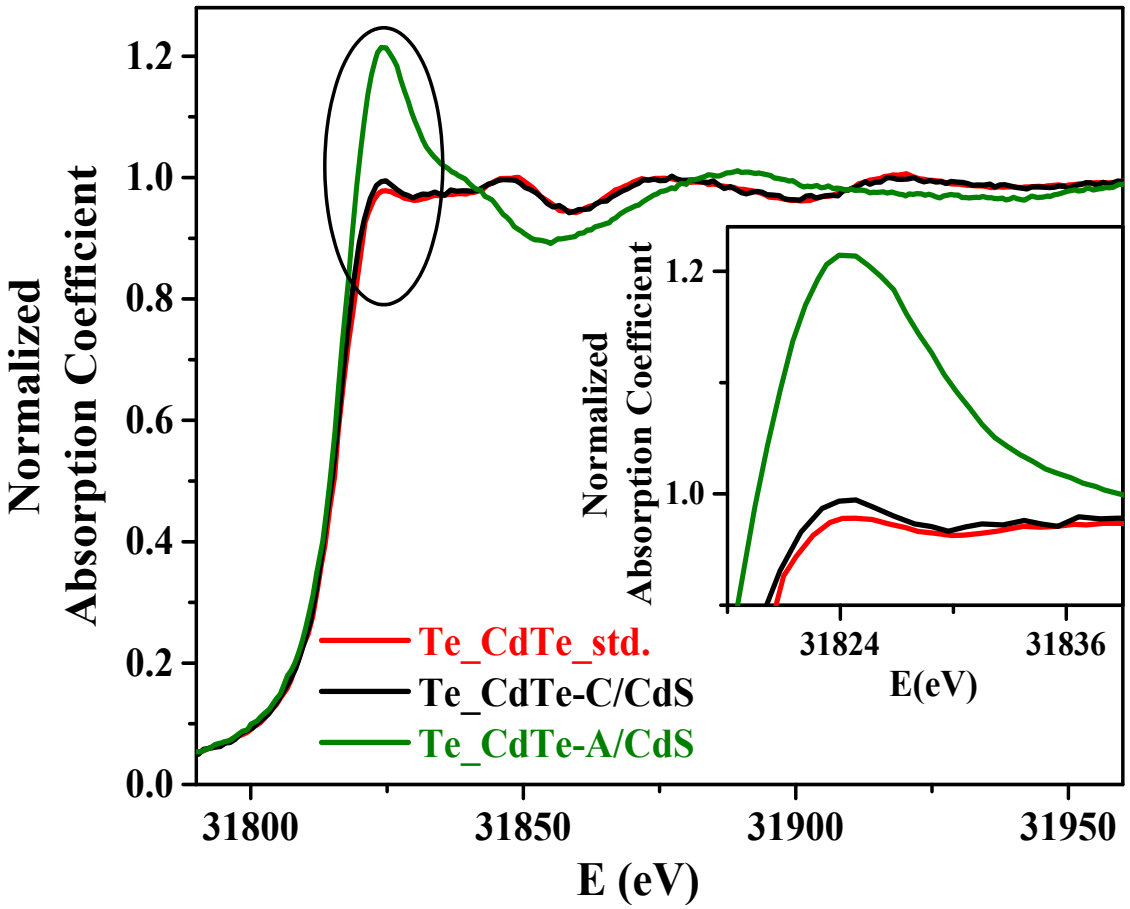

Figure S3. Te edge X-ray Absorption Near Edge Structure (XANES) of both CdTe/CdS core/shell and alloy quantum dots.

The white line for the Te edge of the alloy sample is higher than the Te edge of CdTe standard sample because this sample is slightly oxidized as shown in the table of fit parameters since some of the Te atoms of the alloy are on the surface.

Table S1. List of fit parameters obtained from modeling the data for Cd and Te edges.

Edge	Sample Name	Paths	Bond length R (Å)	Coordination Number (n)	Debye Waller Factor	Energy Shift ΔE (eV)
Cd edge S_o^2**=0.97**	**CdTe-A/CdS** R=1.0-4.5 Å k= 3.3-12.0 Å^{-1}	Cd-S	2.50 ± 0.01	4.1 ± 0.3	0.009 ± 0.001	-1.7 ± 0.7
		Cd-Cd	4.14± 0.03	5.6 ± 3.8	0.02 ± 0.01	
	CdTe-C/CdS R=1.2-3 Å k= 3.4-10.4 Å^{-1}	Cd-S	2.48 ± 0.01	4.5 ± 0.8	0.016 ± 0.002	-4.2 ± 1.0
		Cd-Te	2.77 ± 0.01	1.3 ± 0.3	0.008 ± 0.002	
Te edge S_o^2**=0.98**	**CdTe-A/CdS** R=1.0-3.2 Å k= 2.7-9.3 Å^{-1}	Te-O	1.90 ± 0.02	2.3 ± 0.3	0.003 ± 0.002	7.6 ± 1.4
		Te-Cd	2.79 ± 0.03	1.2 ± 0.3	0.007	
	CdTe-C/CdS R=1-4.8 Å k= 3.1-9.0 Å^{-1}	Te-Cd	2.77 ± 0.01	3.6 ± 0.4	0.008 ± 0.002	3.7 ± 0.9
		Te-Te	4.51 ± 0.06	12	0.03 ± 0.01	

Table S2. Theoretical bond lengths generated using FEFF and used for fit.

Path	Bond Length (Å)	Coordination Number
TeO2 (Te-O)	1.90	2
CdS (Cd-S1)	2.52	1
CdS (Cd-S2)	2.53	3
CdS (Cd-Cd1)	4.12	6
CdS (Cd-Cd2)	4.13	6
CdTe (Cd-Te)	2.81	4
CdTe (Cd-Cd)	4.58	12
CdTe (Te-Cd)	2.81	4
CdTe (Te-Te)	4.58	12