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ZnS/CdX (X = S, Se, Te) core/shell nanowires: An attempt at fine-tuning electronic bandgaps and SQ efficiencies

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Table S1. The static dielectric constants and the energy spectrum for negative values of real part of dielectric constants in the perpendicular and parallel cases, for all the pristine and c/s NWs.

Nanowire	Perpendicular Optical Vector		Parallel Optical Vector	
	$\varepsilon_{\perp}(0)$	Energy range for $\varepsilon_{\parallel}(\omega) < 0$	$\varepsilon_{\parallel}(0)$	Energy range for $\varepsilon_{\parallel}(\omega) < 0$
ZnS	2.70	8.42 eV – 9.32 eV	2.51	8.66 eV – 9.36 eV
CdS	2.53	8.14 eV – 8.72 eV	2.32	8.26 eV – 8.76 eV
CdSe	2.73	7.72 eV – 8.38 eV	2.45	7.84 eV – 8.40 eV
CdTe	2.98	6.64 eV – 7.66 eV	2.76	6.68 eV – 8.16 eV
ZnS/CdS	2.69	8.18 eV – 8.94 eV	2.47	8.58 eV – 9.00 eV
ZnS/CdSe	3.42	– –	2.69	8.90 eV – 9.40 eV
ZnS/CdTe	4.23	8.54 eV – 8.80 eV	3.21	6.94 eV – 8.94 eV

Table S2. The static refractive indices and the maximum refractive indices of the pristine and c/s NWs, for both the parallel and perpendicular optical vectors.

Nanowire	Perpendicular Optical Vector		Parallel Optical Vector	
	$n_{\perp}(0)$	$n_{\perp max}(\omega)$	$n_{\parallel}(0)$	$n_{\parallel max}(\omega)$
ZnS	1.64	2.22 at 2.77 eV	1.58	2.12 at 4.47 eV
CdS	1.59	2.06 at 2.15 eV	1.52	1.80 at 4.34 eV
CdSe	1.65	2.20 at 2.02 eV	1.57	1.91 at 3.65 eV
CdTe	1.72	2.33 at 2.21 eV	1.66	2.26 at 3.48 eV
ZnS/CdS	1.64	2.16 at 2.25 eV	1.57	1.98 at 4.36 eV
ZnS/CdSe	1.85	2.29 at 1.56 eV	1.64	1.91 at 3.25 eV
ZnS/CdTe	2.06	2.78 at 2.28 eV	1.79	2.14 at 2.75 eV

Table S3. The maxima of the extinction coefficients and the skin depths, for perpendicular and parallel incidents, of the pristine and c/s NWs.

Nanowire	Perpendicular Optical Vector		Parallel Optical Vector	
	$K_{\perp max}(\omega)$	$\delta_{\perp}$(Å)	$K_{\parallel max}(\omega)$	$\delta_{\parallel}$(Å)
ZnS	1.64	217	1.58	217
CdS	1.59	198	1.52	230
CdSe	1.65	219	1.57	242
CdTe	1.72	278	1.66	378
ZnS/CdS	1.64	192	1.57	234
ZnS/CdSe	1.85	586	1.64	259
ZnS/CdTe	2.06	416	1.79	242

Table S4. The static reflectances and the maximum reflectances of the pristine and c/s NWs, for both the parallel and perpendicular optical vectors.

Nanowire	Perpendicular Optical Vector		Parallel Optical Vector	
	$R_{\perp}(0)$	$R_{\perp max}(\omega)$	$R_{\parallel}(0)$	$R_{\parallel max}(\omega)$
ZnS	5.93%	28.09% at 9.08 eV	5.11%	21.90% at 8.85 eV
CdS	5.22%	32.33% at 8.43 eV	4.29%	22.60% at 8.43 eV
CdSe	6.03%	32.33% at 8.10 eV	4.86%	23.30% at 8.04 eV
CdTe	7.08%	30.38% at 7.13 eV	6.16%	25.04% at 6.89 eV
ZnS/CdS	5.89%	30.71% at 8.39 eV	4.95%	20.24% at 8.72 eV
ZnS/CdSe	8.89%	18.21% at 2.56 eV	5.90%	18.81% at 9.28 eV
ZnS/CdTe	11.95%	29.42% at 2.45 eV	8.04%	25.05% at 7.65 eV