Supporting information for

"A solvent-based atomistic theory for doping colloidal–synthesized quantum dots via cation exchange"

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Table S1 lists the crystal structure and formation energies of 3*d* transition metal selenide and CdSe. We take the total energy of bulk metals ($E_{\mathrm{M}}^{\mathrm{bulk}}$) and selenium ($E_{\mathrm{Se}}^{\mathrm{bulk}}$) as the reference for the chemical potential. So, the chemical potential (μ) can be written as $\mu \equiv E^{\mathrm{bulk}} + \mu^{*}$.

Table S1. The space group, lattice parameters and formation energies of bulk metal selenides. The experimental lattice parameters are listed for comparison.

	Space Group	*a* (Å)		*c* (Å)		$\Delta H_f^{\mathrm{bulk}}$ (eV)
		Expt.	Calc.	Expt.	Calc.	
CdSe [1]	$F\bar{4}3m$	6.08	6.21	--	--	-1.264
VSe [2]	$P6_3mc$	3.58	3.75	5.98	5.83	-0.809
CrSe [2]	$P6_3mc$	3.68	3.78	6.02	6.13	-0.623
MnSe [2]	$Fm\bar{3}m$	5.82	5.40	--	--	-0.664
FeSe [2]	$P6_3mc$	3.63	3.84	5.95	5.03	-0.203
CoSe [2]	$P6_3mc$	3.63	3.62	5.30	5.21	-0.282
NiSe [2]	$P6_3mc$	3.66	3.71	5.35	5.23	-0.498
CuSe [3]	$P6_3/mmc$	3.94	3.95	17.25	17.42	-0.168

The formation energies of bulk metal-selenide were calculated as:

$$\Delta H_f^{\mathrm{bulk}}(\mathrm{MSe}) = E^{\mathrm{bulk}}(\mathrm{MSe}) - E_{\mathrm{M}}^{\mathrm{bulk}} - E_{\mathrm{Se}}^{\mathrm{bulk}}.$$

Considering the equilibrium condition $\mu_{\mathrm{M}} + \mu_{\mathrm{Se}} = \mu_{\mathrm{MSe}}$, we can write the formation energy of bulk metal-selenide as:

$$\mu_{\mathrm{M}}^{*} + \mu_{\mathrm{Se}}^{*} = \Delta H_f^{\mathrm{bulk}}(\mathrm{MSe}).$$

As discussed in the text, we here consider the Se-rich condition, where μ_{Se}^{*} reaches its upper limit ($\mu_{\mathrm{Se}}^{*} = 0$) and $\mu_{\mathrm{Cd}}^{*} = -1.264$ eV. Similarly, under Se-rich condition, $\mu_{\mathrm{TM}}^{*} = \Delta H_f^{\mathrm{bulk}}(\mathrm{TMSe})$.

Reference

1. Samarth, N.; Luo, H.; Furdyna, J. K.; Qadri, S. B.; Lee, Y. R.; Ramdas, A. K.; Otsuka, N., Growth of Cubic (Zinc Blende) CdSe by Molecular Beam Epitaxy. *Applied Physics Letters* **1989**, *54*, 2680-2682.

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