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SUPPORTING INFORMATION

Ligand-stabilized CdSe Nanoplatelet Hybrid Structures with Tailored Geometric and Electronic Properties. New Insights from theory

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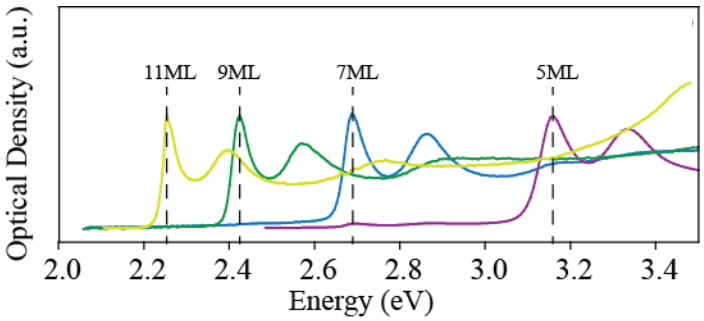

Figure S1. Absorption spectra of the 5, 7, 9 and 11 atomic layers (MLs) thick CdSe zinc blende nanoplatelets passivated by carboxylic acids.

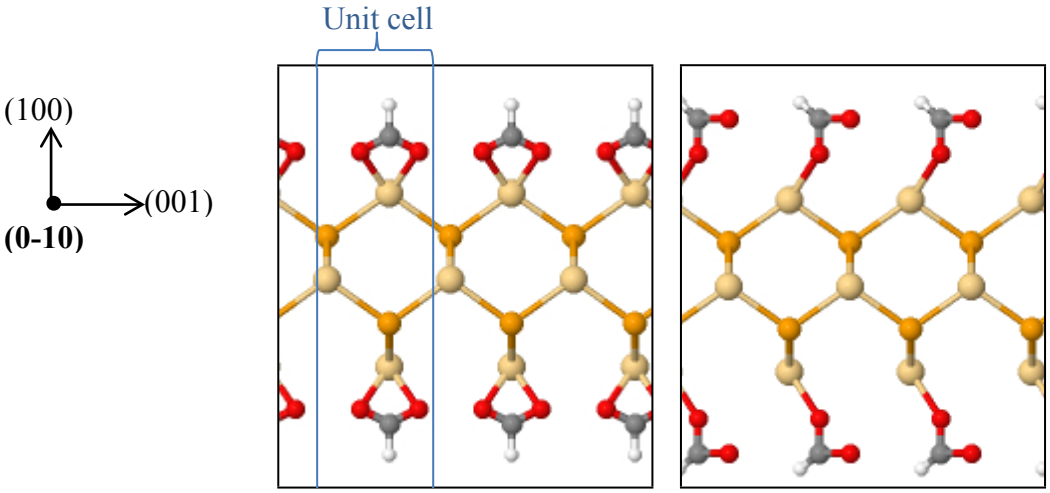

Figure S2. Initial geometries of CdSe.HCOO with a) bidentate and b) monodentate adsorption mode of the $HCOO^-$ ligand.

Table S1. Computed Mulliken atomic charges (in $|e^-|$) for 5 and 13 layers thick CdSe zinc blende slabs with $HCOO^-$, OH^- or SH^- ligands adsorbed on both of its [100] basal planes. Cd and Se atoms are indicated as Cd_n and Se_n where n=1-13 and n is the number of atomic layers, n=1 and n=5 (13) being the outermost layer of the slab. The atoms in equivalent positions with respect to the (100) surfaces are shown in parentheses.

CdSe.HCOO			
	5 layers		***13 layers***
Cd_{1a} (Cd_{5a})	+0.882	**Cd_{1a} (Cd_{13a})**	+0.880
Cd_{1b} (Cd_{5b})	+0.882	**Cd_{1b} (Cd_{13b})**	+0.880
Se_{2a} (Se_{4a})	-0.434	**Se_{2a} (Se_{12a})**	-0.430
Se_{2b} (Se_{4b})	-0.434	**Se_{2b} (Se_{12b})**	-0.430
Cd_{3a}	+0.430	**Cd_{3a} (Cd_{11a})**	+0.426
Cd_{3a}	+0.430	**Cd_{3a} (Cd_{11a})**	+0.426
O_1	-0.485	**Se_{4a} (Se_{10a})**	-0.427
O_2	-0.610	**Se_{4a} (Se_{10a})**	-0.427
C	+0.293	**Cd_5 (Cd_9)**	+0.424
H	+0.140	**Se_6 (Se_8)**	-0.427
		Cd_7	+0.423
		O_1	-0.485
		O_2	-0.611
		C	+0.293
		H	+0.140
CdSe.SH			
	5 layers		***13 layers***
Cd_{1a} (Cd_{5a})	+0.342	**Cd_{1a} (Cd_{13a})**	+0.341
Cd_{1b} (Cd_{5b})	+0.348	**Cd_{1b} (Cd_{13b})**	+0.348
Se_{2a} (Se_{4a})	-0.436	**Se_{2a} (Se_{12a})**	-0.435
Se_{2b} (Se_{4b})	-0.448	**Se_{2b} (Se_{12b})**	-0.446
Cd_{3a}	+0.448	**Cd_{3a} (Cd_{11a})**	+0.431
Cd_{3b}	+0.448	**Cd_{3b} (Cd_{11b})**	+0.440

S_1	-0.098	**Se_{4a} (Se_{10a})**	-0.423
S_2	-0.116	**Se_{4a} (Se_{10a})**	-0.423
H_1	-0.052	**Cd_5 (Cd_9)**	+0.423
H_2	+0.013	**Se_6 (Se_8)**	-0.424
		Cd_7	+0.422
		S_1	-0.097
		S_2	-0.118
		H_1	-0.049
		H_2	+0.013

CdSe.OH			
	5 layers		***13 layers***
Cd_{1a} (Cd_{5a})	+0.857	**Cd_{1a} (Cd_{13a})**	+0.856
Cd_{1b} (Cd_{5b})	+0.857	**Cd_{1b} (Cd_{13b})**	+0.856
Se_{2a} (Se_{4a})	-0.434	**Se_{2a} (Se_{12a})**	-0.429
Se_{2b} (Se_{4b})	-0.434	**Se_{2b} (Se_{12b})**	-0.429
Cd_{3a}	+0.441	**Cd_{3a} (Cd_{11a})**	+0.432
Cd_{3b}	+0.441	**Cd_{3b} (Cd_{11b})**	+0.432
O	-0.949	**Se_{4a} (Se_{10a})**	-0.427
H	+0.306	**Se_{4a} (Se_{10a})**	-0.427
		Cd_5 (Cd_9)	+0.424
		Se_6 (Se_8)	-0.422
		Cd_7	+0.422
		O	-0.950
		H	+0.306

Table S2. Number of electrons on Cd, S and O atomic orbitals of 5 layers thick CdSe zinc blende slabs with $HCOO^-$, OH^- or SH^- ligands adsorbed on both of its [100] basal planes. All values are expressed in $|e^-|$.

			CdSe.HCOO				
Cd_1	**4sp**	**4d**	**5sp**	**5d**	**6sp**	**6d**	**7sp**
	4.171	5.820	0.908	3.224	0.248	0.998	3.750
O_1	**1sp**	**2sp**	**3sp**	**3d**	**4sp**		
	1.998	2.715	2.660	0.024	1.087		
O_2	**1sp**	**2sp**	**3sp**	**3d**	**4sp**		
	1.999	2.714	2.698	0.020	1.179		
			CdSe.SH				
Cd_{1a}	**4sp**	**4d**	**5sp**	**5d**	**6sp**	**6d**	**7sp**
	4.181	5.797	0.851	3.204	0.852	1.031	3.742
Cd_{1b}	**4sp**	**4d**	**5sp**	**5d**	**6sp**	**6d**	**7sp**
	4.181	5.797	0.862	3.203	0.835	1.032	3.742
S_1	**1s**	**2s+2p**	**3s+3p**	**3d**	**4s+4p**	**5s+5p**	
	2.010	4.759	3.313	0.049	5.295	0.672	
S_2	**1s**	**2s+2p**	**3s+3p**	**3d**	**4s+4p**	**5s+5p**	
	2.010	4.759	3.313	0.049	5.293	0.692	
			CdSe.OH				
Cd_1	**4sp**	**4d**	**5sp**	**5d**	**6sp**	**6d**	**7sp**
	4.171	5.815	0.826	3.223	0.365	0.993	3.750
O	**1sp**	**2sp**	**3sp**	**3d**	**4sp**		
	1.998	2.682	2.737	0.016	1.516		