Supporting Information:

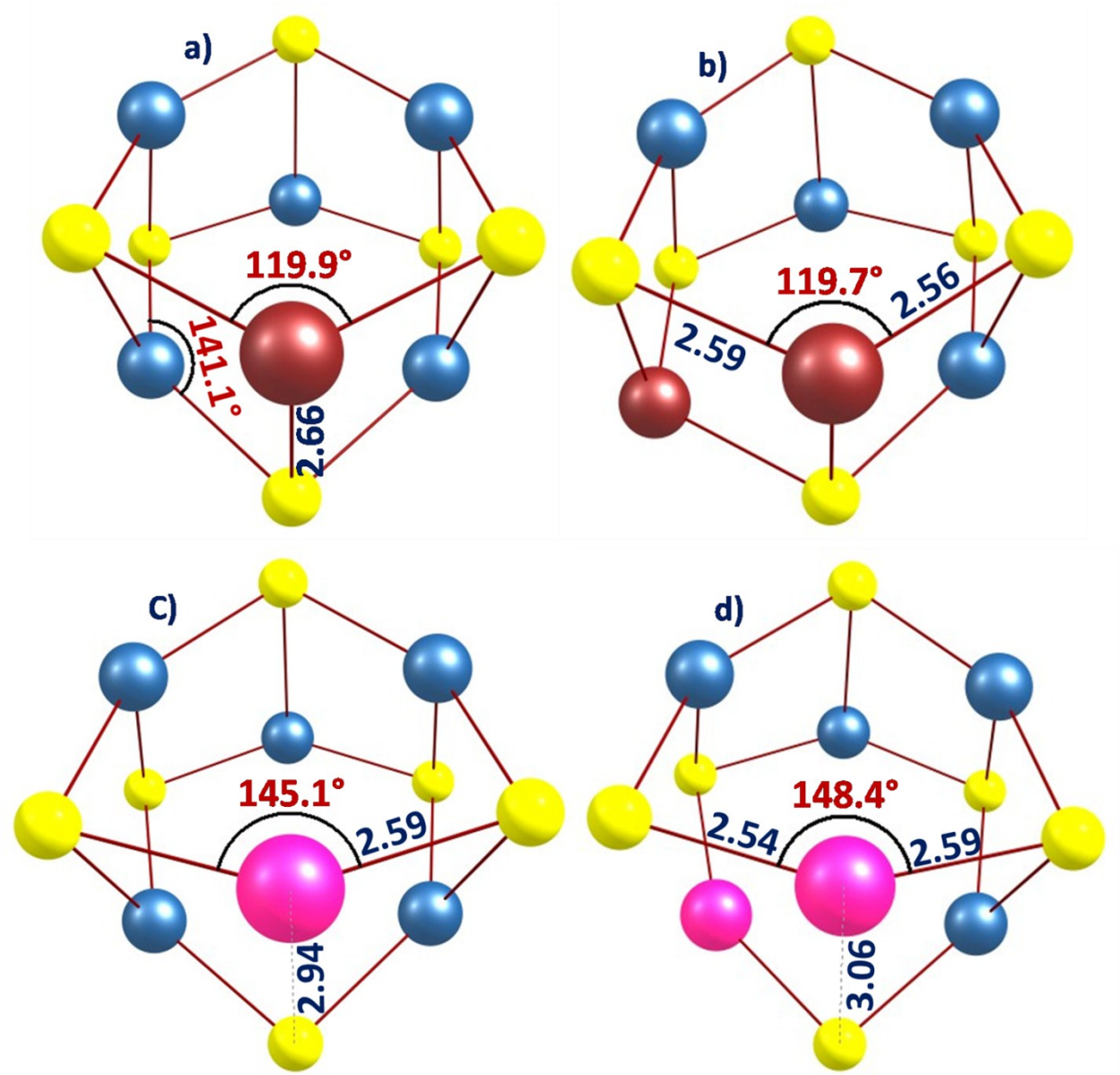

Figure S1. The optimized structures of doped $Cd_{6-y}X_yS_6$ (X= In^{2+}, Hg^{2+};y= 1, 2) clusters. The significant distorted bond lengths (in Å) are denoted in navy and bond angles (in ˚) are in dark red. Cd atoms are in blue, S in dark yellow, In in brown, and Hg in dark pink.

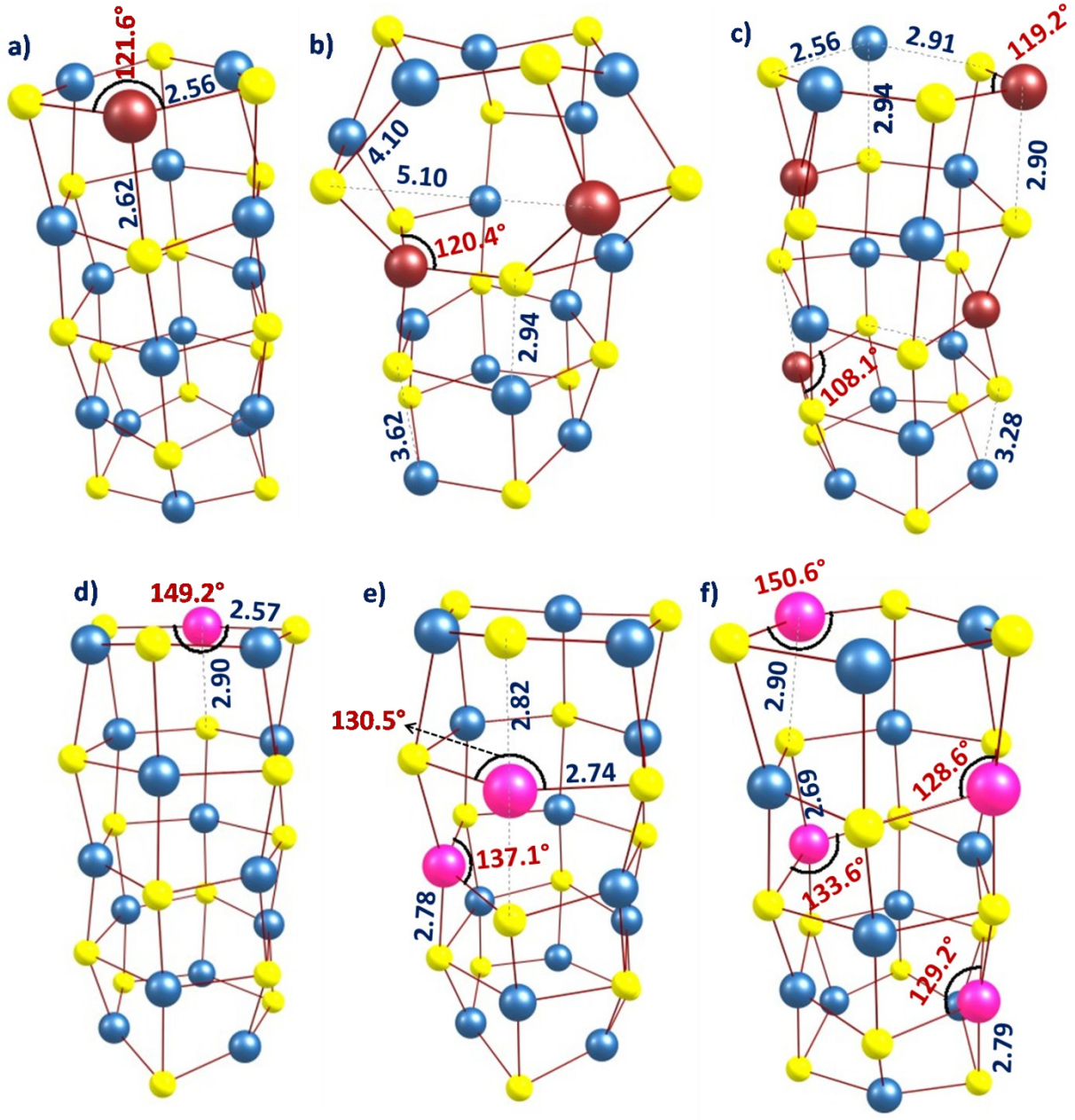
a)
121.6°
2.56
2.62
b)
4.10
5.10
120.4°
2.94
3.62
c)
2.56
2.91
119.2°
2.94
2.90
108.1°
3.28
d)
149.2°
2.57
2.90
e)
130.5°
2.82
2.74
137.1°
2.78
f)
150.6°
2.90
2.69
128.6°
133.6°
129.2°
2.79

Figure S2. The optimized structures of doped $Cd_{15-y}X_yS_{15}$ (X= In^{2+}, Hg^{2+};y= 1, 2, 4) clusters. The significant distorted bond lengths (in Å) are denoted in navy and bond angles (in ˚) are in dark red. Cd atoms are in blue, S in dark yellow, In in brown, and Hg in pink.

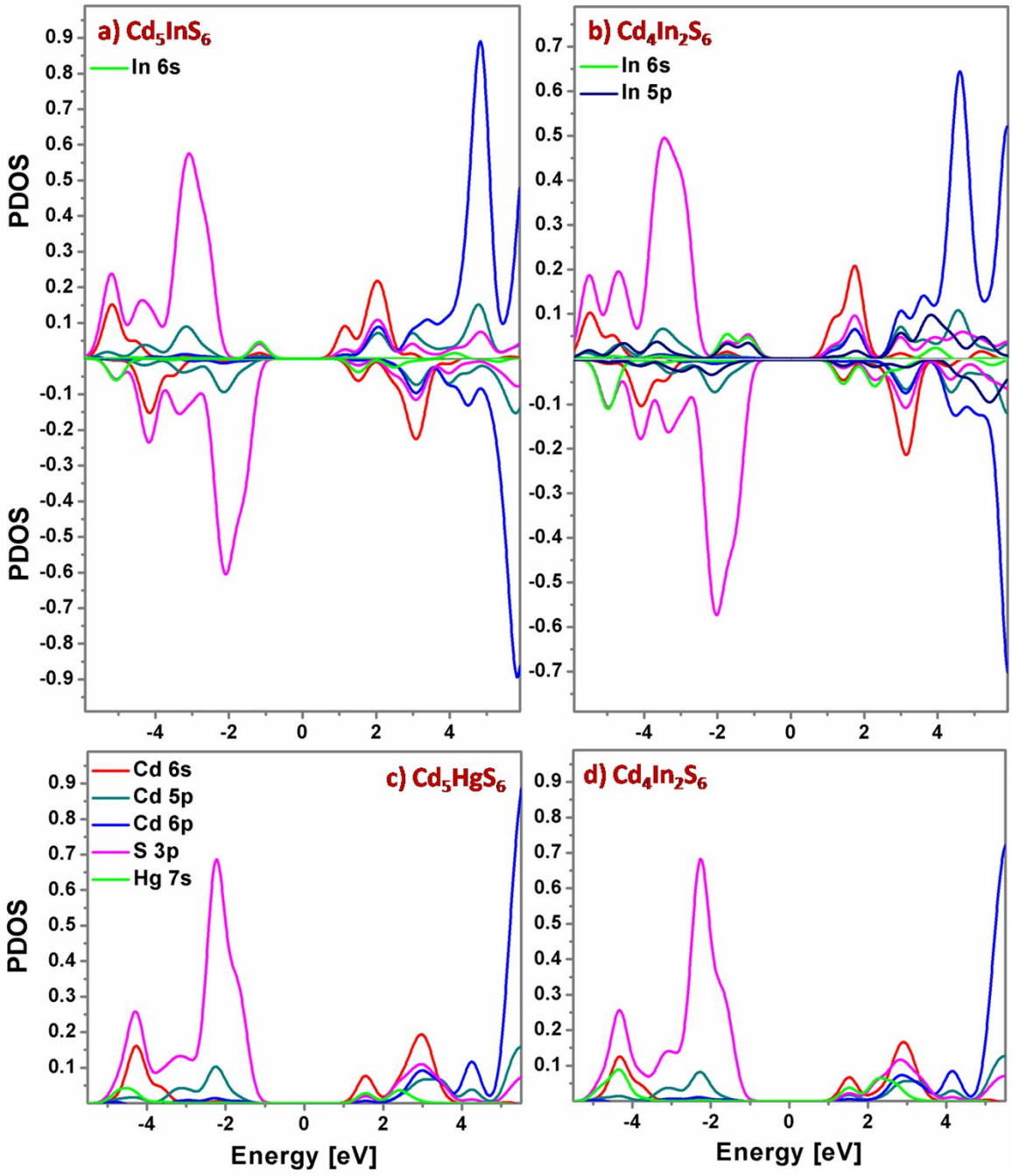

Figure S3. The calculated Total (TDOS) and partial (PDOS) density of states for the doped $Cd_{6-y}X_yS_6$ (X= In, Hg and y=1, 2) clusters. The positive and negative amplitudes represent the spin up and spin down states of the doped clusters respectively. The midgap is set to zero.

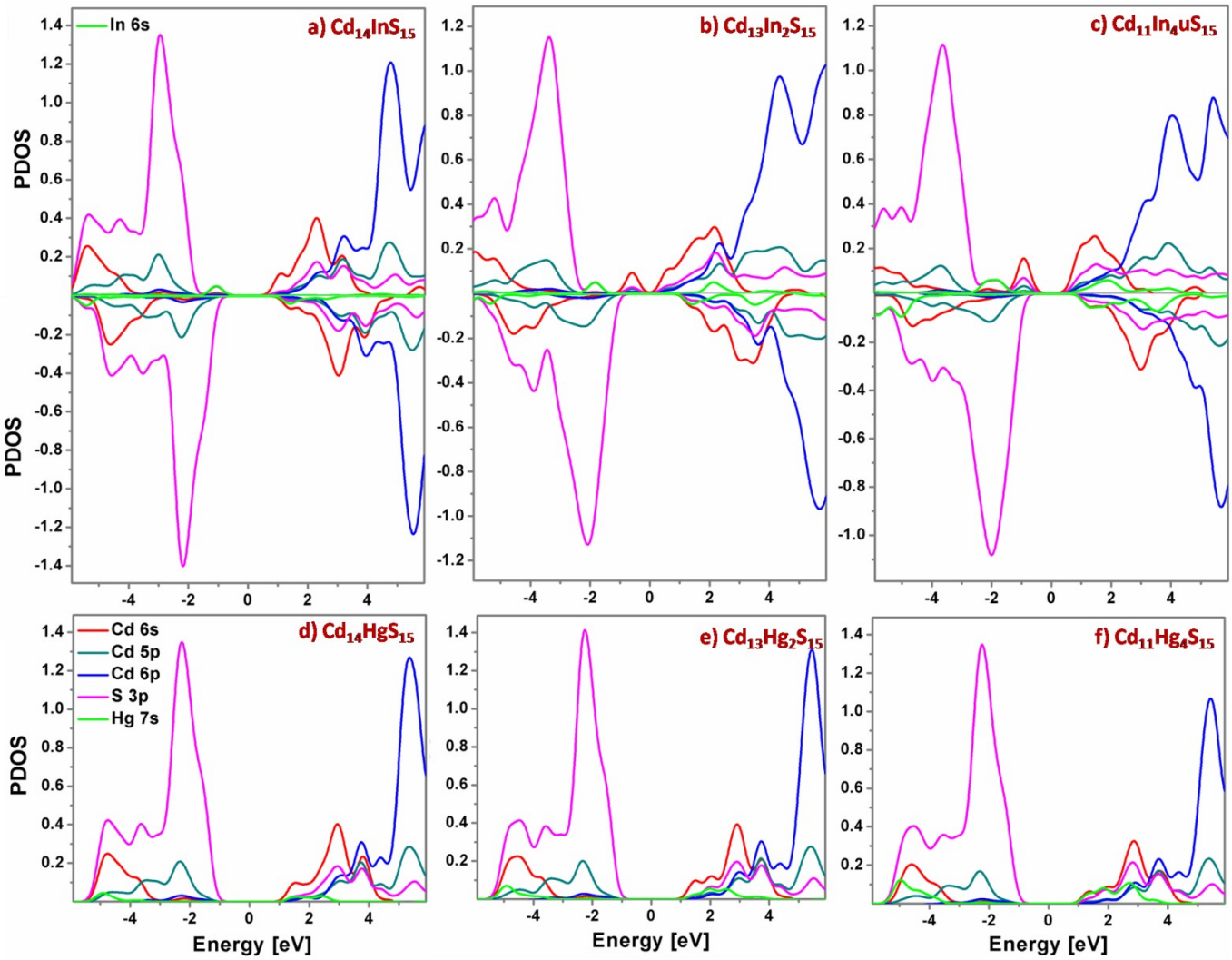

Figure S4. The calculated Total (TDOS) and partial (PDOS) density of states for the doped $Cd_{15-y}X_yS_{15}$ (X= In, Hg and y=1, 2 and 4) clusters. The positive and negative amplitudes represent the spin up and spin down states of the doped clusters respectively. The midgap is set to zero.

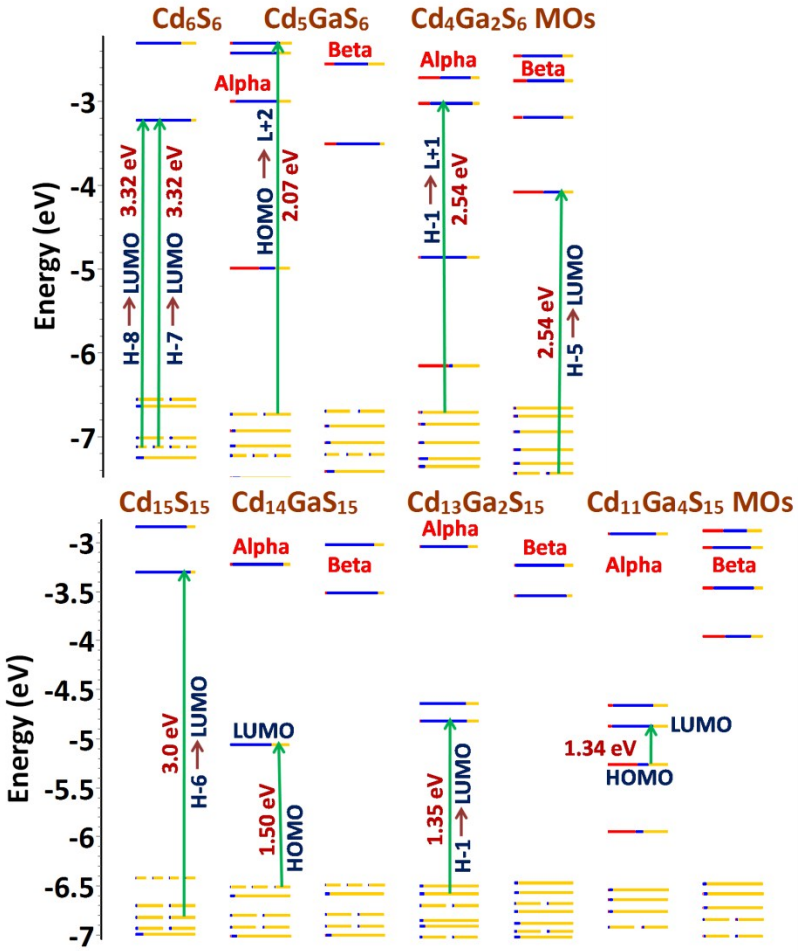

Figure S5. The energy levels of MOs near HOMO and LUMO of both Cd_6S_6 and $Cd_{15}Se_{15}$ clusters doped with Ga^{2+} along with their composition due to the AOs are indicated by dark blue for Cd^{2+}, yellow for S^{2-} and red for Ga^{2+} ions. The green arrows represent the singlet transitions calculated using TD-DFT.

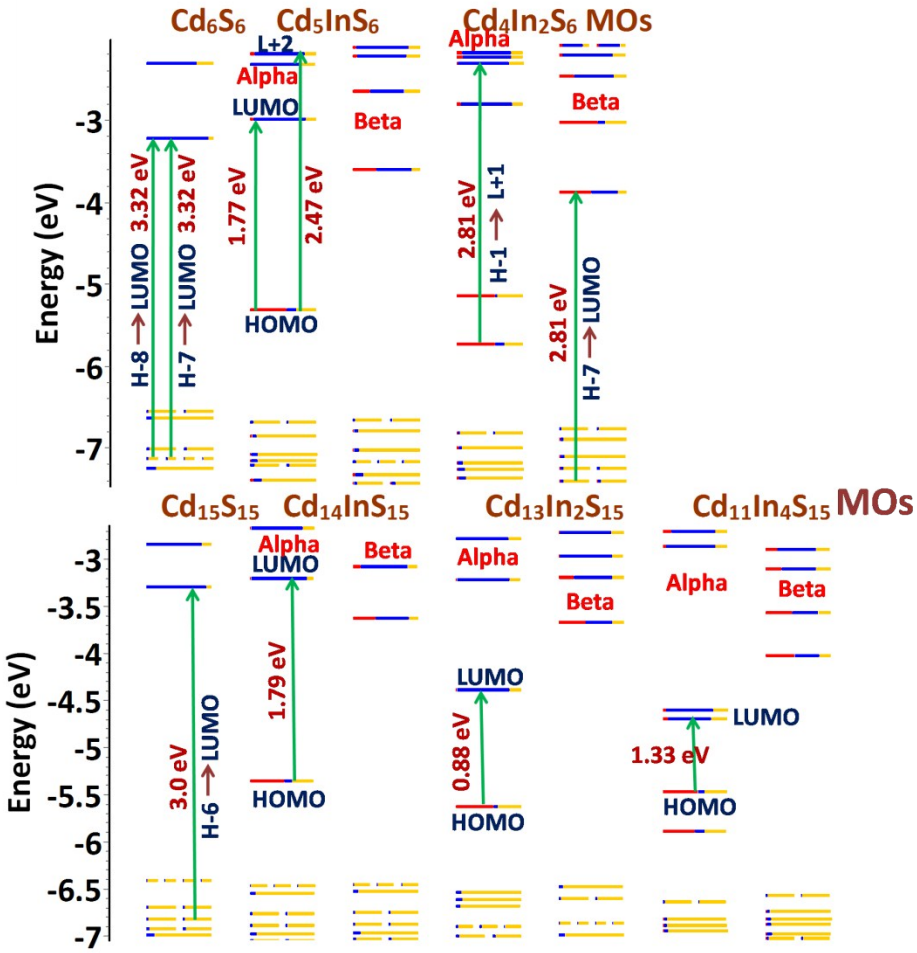

Figure S6. The energy levels of MOs near HOMO and LUMO of both Cd_6S_6 and $Cd_{15}Se_{15}$ clusters doped with In^{2+} along with their composition due to the AOs are indicated by dark blue for Cd^{2+}, yellow for S^{2-} and red for In^{2+} ions. The green arrows represent the singlet transitions calculated using TD-DFT.

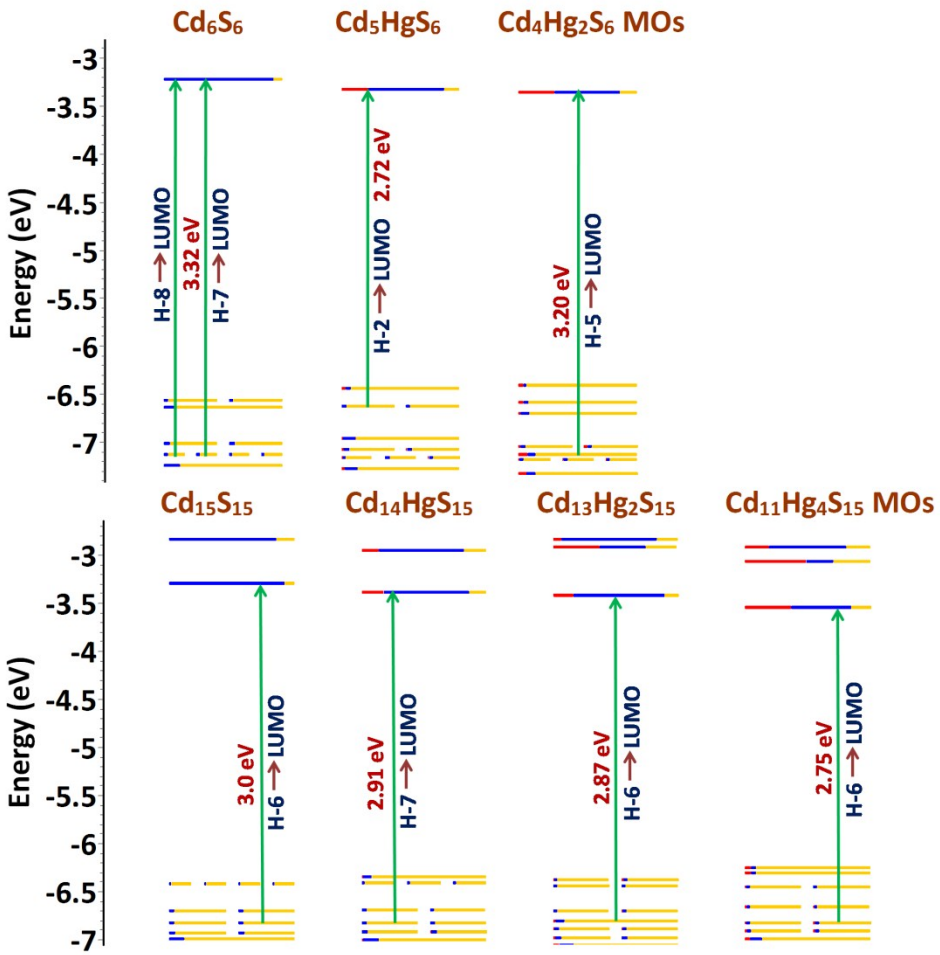

Figure S7. The energy levels of MOs near HOMO and LUMO of both Cd_6S_6 and $Cd_{15}Se_{15}$ clusters doped with Hg^{2+} along with their composition due to the AOs are indicated by dark blue for

Cd^{2+}, yellow for S^{2-} and red for Hg^{2+} ions. The green arrows represent the singlet transitions calculated using TD-DFT.

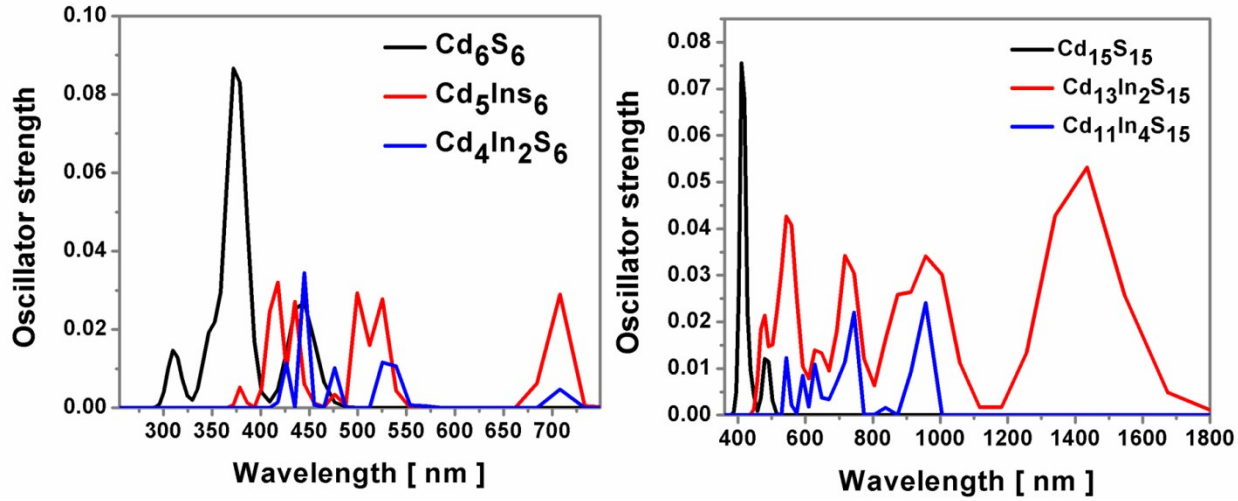

Figure S8. The absorption spectra of $Cd_{6-y}In_yS_6$ clusters where y = 1, 2 are compared with pure Cd_6S_6 cluster calculated using TD-DFT.

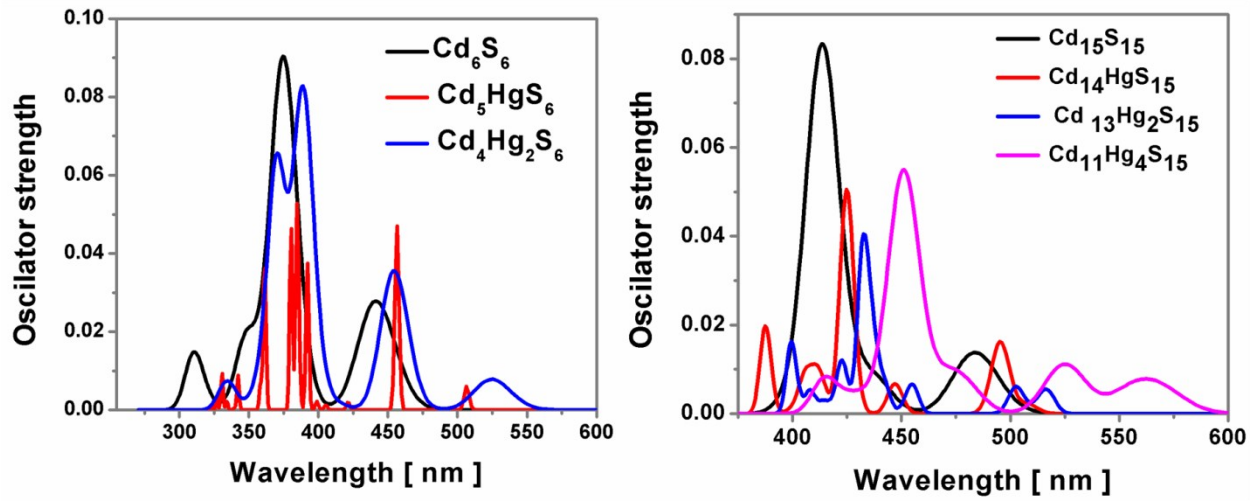

Figure S9. The absorption spectra of Cd_6S_6 and $Cd_{6-y}Hg_yS_6$ clusters where y = 1, 2 were calculated using TD-DFT when the impurity is located at the surface.

Table S1. Dopant's binding energy (E_b), HOMO-LUMO gap (E_g), Natural atomic charge (q_X) and spin density (ρ_X) of dopants for the pristine $Cd_{15}S_{15}$ and doped $Cd_{15-y}X_yS_{15}$ (y=1, 2, 4) clusters. The spin multiplicity (2S+1) is given in parentheses.

system	E_b [eV]	Eg [eV]	q_X [a.u.]	$\rho_{(X)}$
$Cd_{15}S_{15}$ (1)	-	3.11	-	-
Cu (2)	0.85	1.55	0.46	0.08
Cu_2 (3)	1.67	1.81	[0.46/0.50]*	0.17[0.08/0.09]
Cu_4 (5)	2.74	0.76	[0.39/0.39/0.43/0.33]	0.48[0.19/0.06/0.07/0.16]
Ga (2)	1.43	1.55	1.0	0.19
Ga_2 (3)	2.56	1.09	[1.23/1.24]	1.23[0.61/0.62]*
Ga_4 (5)	5.37	0.70	[1.0/1.71/1.19/0.95]	1.47[0.16/0.59/0.59/0.13]
In (2)	1.32	1.73	1.15	0.24
In_2 (3)	2.76	0.71	[1.12/1.46]	0.93[0.21/0.72]
In_4 (5)	4.38	0.58	[1.14/1.44/1.47/1.13]	1.88[0.23/0.71/0.72/0.22]
Hg (1)	-1.28	2.96	1.01	0
Hg_2 (1)	-2.95	2.95	[1.02/1.04]	0
Hg_4 (1)	-5.69	2.70	[1.01/1.02/1.05/1.02]	0

*the natural atomic charge and spin density at individual dopants.

Table S2. The calculated absorption energy (E in eV and λ in nm) and oscillator strength (f in a.u.) of bare $Cd_{15}Se_{15}$ cluster doped by a variety of dopants at TD-B3LYP/Lanl2dz/6-31+G* level of theory.

system	Absorption energy (E) [eV]	Absorption wavelength (λ) [nm]	Orbital transitions	Oscillator strength f(a.u.)
$Cd_{15}S_{15}$	3.00	412.88	H-6 ->LUMO(0.67)$^{\$}$	0.083
$Cd_{14}CuS_{15}$	1.83	676.035	H-8 (b)* ->LUMO(b)(0.87)	0.048
$Cd_{14}CuS_{15}$	2.27	545.876	H-14 (b) ->LUMO(b)(0.68)	0.023
$Cd_{14}CuS_{15}$	1.83	676.663	H-18 (b) ->LUMO(b)(0.45)	0.011
$Cd_{13}Cu_2S_{15}$	1.59	778.311	H-8 (b) ->LUMO(b)(0.52)	0.045
			H-9 (b) ->LUMO(b)(0.47)	0.045
$Cd_{13}Cu_2S_{15}$	1.50	825.740	H-1 (b) ->L+1(b) (0.57)	0.021
$Cd_{11}Cu_4S_{15}$	1.07	1164.724	H-7 (b) ->LUMO(b)(0.38)	0.008
$Cd_{14}GaS_{15}$	1.76	705.181	HOMO (a) ->L+1(a) (0.96)	0.041
$Cd_{14}GaS_{15}$	1.50	828.665	HOMO (a) ->LUMO (a) (0.97)	0.044
$Cd_{13}Ga_2S_{15}$	1.48	839.210	H-1 (a)* ->LUMO(a) (0.96)	0.028
$Cd_{13}Ga_2S_{15}$	1.35	916.777	H-1 (a) ->LUMO(a) (0.87)	0.069
$Cd_{11}Ga_4S_{15}$	1.34	926.713	HOMO (a) ->LUMO(a) (0.80)	0.044
$Cd_{14}InS_{15}$	1.79	692.885	HOMO (a) ->LUMO(a) (0.97)	0.039

$Cd_{13}In_2S_{15}$	1.70	730.741	H-1 (a) ->LUMO(a) (0.72)	0.080
$Cd_{13}In_2S_{15}$	0.88	1405.565	HOMO (a) ->LUMO(a) (1.00)	0.055
$Cd_{11}In_4S_{15}$	1.33	930.538	HOMO (a) ->LUMO(a) (0.69)	0.034
$Cd_{14}HgS_{15}$	2.91	426.071	H-6 (a) ->LUMO(a) (0.55)	0.071
$Cd_{14}HgS_{15}$	2.92	424.112	H-6 (a) ->LUMO(a) (0.60)	0.047
$Cd_{14}HgS_{15}$	2.91	425.553	H-7 (a) ->LUMO(a) (0.59)	0.063
$Cd_{13}Hg_2S_{15}$	2.85	435.187	H-6 (a) ->LUMO(a) (0.60)	0.039
$Cd_{13}Hg_2S_{15}$	2.87	431.582	H-6 (a) ->LUMO(a) (0.49)	0.035
$Cd_{11}Hg_4S_{15}$	2.75	450.183	H-6 (a) ->LUMO(a) (0.62)	0.052

*a,b refers to alpha and beta MOs,

$Values given with in parenthesis are the orbital coefficient.

For information only the transitions with oscillator strength higher than 0.008 a.u. are given.

Cartesian coordinates for the optimized structures in standard orientation:

For bare Cd_6S_6 and doped Cd_6XS_6 clusters:

1. **Bare Cd_6S_6 cluster:**

****

48 2.234010 -0.186590 -1.220035

16 1.572997 2.265675 -1.449828

48 -0.955935 2.027046 -1.219165

16 -2.750692 0.229914 -1.449138

48 -1.279345 -1.840601 -1.219051

16 1.175177 -2.494975 -1.449963

48 0.955932 -2.027031 1.219165

16 -1.572998 -2.265677 1.449834

48 -2.234002 0.186591 1.220027

16 -1.175179 2.494979 1.449966

48 1.279337 1.840584 1.219056

16 2.750702 -0.229914 1.449138

****

2. Cd_5CuS_6 cluster:

****

29 -0.000010 1.842851 1.461808

16 2.238198 1.348957 1.690853

48 1.900900 -1.123574 1.141913

16 0.000016 -2.820435 1.101090

48 -1.900883 -1.123593 1.141916

16 -2.238213 1.348935 1.690855

48 -1.995283 1.391276 -0.954344

16 -2.397271 -1.037756 -1.560867

48 0.000010 -1.910786 -1.458167

16 2.397281 -1.037729 -1.560870

48 1.995265 1.391297 -0.954344

16 -0.000018 2.983999 -0.761512

****

3. $Cd_4Cu_2S_6$ cluster:

****

29 -0.764685 1.870095 1.270018

16 1.409302 2.582815 1.012279

48 2.388042 0.235180 0.903293

16 1.583129 -2.148280 1.226123

48	-0.915045	-1.640406	1.373244
16	-2.413196	0.391595	1.785618
48	-2.388042	0.235181	-0.903293
16	-1.583129	-2.148280	-1.226123
48	0.915045	-1.640406	-1.373244
16	2.413196	0.391595	-1.785618
29	0.764686	1.870095	-1.270018
16	-1.409301	2.582816	-1.012279

****

4. **Cd_5GaS_6 cluster:**

****

31	-2.479092	0.000884	1.411508
16	-1.361983	2.085121	1.631967
48	1.161421	1.880082	1.199492
16	2.877116	-0.001004	1.224342
48	1.160062	-1.880849	1.199491
16	-1.363464	-2.084149	1.632018
48	-1.309978	-1.923707	-1.056710
16	1.144005	-2.377407	-1.484872
48	2.083637	-0.000725	-1.368941
16	1.145718	2.376635	-1.484881
48	-1.308566	1.924548	-1.056763
16	-2.997878	0.001044	-1.003078

****

5. **$Cd_4Ga_2S_6$ cluster:**

****

31	-0.967491	2.154682	2.077522
16	0.685030	2.703300	0.576452
48	3.020351	0.638916	0.524627
16	1.956235	-1.786347	1.151898
48	-0.526054	-1.686383	1.601050
16	-2.259199	0.270296	1.917291
48	-2.477127	-0.160798	-0.786694
16	-1.479279	-2.487377	-0.756710
48	0.937482	-1.699389	-1.252867
16	1.841139	0.549690	-2.184350
31	0.116515	1.769311	-1.452672
16	-1.959116	1.870662	-2.173581

****

6. **Cd_5HgS_6 cluster:**

****

80	-2.188232	-0.000884	-0.885889
16	-1.436909	-2.469719	-1.085306
48	1.065213	-1.971883	-1.305128
16	2.591555	0.000986	-1.843288
48	1.063523	1.972565	-1.305213
16	-1.438964	2.468587	-1.085430
48	-0.711222	1.913914	1.509487
16	1.789299	2.388731	1.266371
48	2.595965	0.001039	0.878538

16 1.791295 -2.387322 1.266493

48 -0.709558 -1.914296 1.509591

16 -2.266884 -0.000857 2.048777

****

7. **$Cd_4Hg_2S_6$ cluster:**

****

80 -1.571724 1.371338 -1.132210

16 -2.184794 -0.990203 -1.846466

48 0.196344 -1.846850 -1.784767

16 2.585626 -0.918628 -1.775586

48 2.198090 1.427512 -0.842896

16 0.274337 3.111633 -0.634746

48 0.196260 1.846859 1.784766

16 2.585584 0.918741 1.775586

48 2.198152 -1.427417 0.842897

16 0.274475 -3.111622 0.634744

80 -1.571661 -1.371406 1.132208

16 -2.184838 0.990104 1.846473

****

8. **Cd_5InS_6 cluster:**

****

49 -2.672493 -0.004386 -1.094773

16 -1.414584 -2.215287 -1.347602

48 1.118309 -1.891753 -1.283583

16 2.789870 0.004190 -1.583176

48 1.111412 1.893926 -1.284322

16 -1.422186 2.210825 -1.348438

48 -0.999855 1.905978 1.283635

16 1.494393 2.375529 1.370385

48 2.399616 0.004026 1.108141

16 1.502497 -2.370533 1.371330

48 -0.993038 -1.907941 1.284305

16 -2.674812 -0.003999 1.565717

****

9. **$Cd_4In_2S_6$ cluster:**

****

49 2.220089 1.412237 1.119694

16 2.247093 -1.143267 1.513351

48 -0.124040 -2.059453 1.380404

16 -2.535200 -1.294984 1.526934

48 -2.047817 1.176379 1.156067

16 0.008069 2.688931 1.232339

48 -0.121075 2.059937 -1.380402

16 -2.533233 1.298524 -1.526491

48 -2.050358 -1.173811 -1.155878

16 0.003820 -2.688786 -1.232292

49 2.217672 -1.415374 -1.119960

16 2.248674 1.140035 -1.513603

****

For bare $Cd_{15}S_{15}$ and doped $Cd_{15}XS_{15}$ clusters:

1. **$Cd_{15}S_{15}$ cluster:**

****

48	-5.240075	2.090767	0.599898
16	-5.415162	0.671360	2.696226
48	-5.235499	-1.565518	1.511354
16	-5.413602	-2.671238	-0.765799
48	-5.238252	-0.527797	-2.112470
16	-5.416152	1.997842	-1.930443
48	-2.690392	1.815232	-1.752303
16	-2.643587	-0.679427	-2.721491
48	-2.688396	-2.424153	-0.694727
16	-2.643896	-2.019218	1.949248
48	-2.688770	0.611315	2.446138
16	-2.645189	2.697253	0.773233
48	0.000000	2.320503	0.664597
16	0.000000	0.689465	2.754286
48	0.000000	-1.735560	1.677004
16	0.000000	-2.728251	-0.780967
48	0.000000	-0.583530	-2.338830
16	0.000000	2.042327	-1.970916
48	2.690392	1.815232	-1.752302
16	2.643587	-0.679427	-2.721490
48	2.688396	-2.424152	-0.694727
16	2.643895	-2.019218	1.949248
48	2.688770	0.611315	2.446136

16	2.645189	2.697255	0.773233
48	5.240076	2.090767	0.599898
16	5.415162	0.671360	2.696226
48	5.235499	-1.565519	1.511355
16	5.413602	-2.671238	-0.765799
48	5.238253	-0.527797	-2.112470
16	5.416152	1.997841	-1.930443

****

2. **$Cd_{14}CuS_{15}$ cluster:**

****

48	-5.362145	1.842002	-0.848604
16	-5.415837	2.247599	1.652611
29	-5.101246	0.000021	2.056740
16	-5.415837	-2.247564	1.652650
48	-5.362150	-1.842019	-0.848573
16	-5.573331	-0.000023	-2.581472
48	-2.860764	-0.000025	-2.401398
16	-2.774435	-2.449547	-1.300996
48	-2.767079	-2.236434	1.367579
16	-2.814061	0.000026	2.850566
48	-2.767077	2.236459	1.367539
16	-2.774434	2.449519	-1.301039
48	-0.152101	2.101965	-1.162617
16	-0.086197	2.451860	1.497249
48	-0.054905	0.000025	2.383948

16	-0.086199	-2.451825	1.497295
48	-0.152103	-2.101983	-1.162577
16	-0.173756	-0.000025	-2.784245
48	2.499223	-0.000024	-2.531084
16	2.483965	-2.434683	-1.387978
48	2.620174	-2.181436	1.255524
16	2.600992	0.000026	2.790526
48	2.620176	2.181458	1.255485
16	2.483967	2.434657	-1.388021
48	5.091315	1.884494	-1.166920
16	5.346291	2.403383	1.303771
48	5.187610	0.000017	2.102815
16	5.346287	-2.403363	1.303815
48	5.091315	-1.884516	-1.166885
16	5.204126	-0.000027	-2.865268

****

3. **$Cd_{13}Cu_2S_{15}$ cluster:**

****

48	5.069013	1.090818	2.074155
16	5.404603	2.768319	0.214650
48	5.305246	1.031615	-1.653687
16	5.508720	-1.453126	-2.125733
48	5.203806	-2.228242	0.265875
16	4.984844	-1.352496	2.625820
29	2.584482	-1.133879	2.023551

16	2.631759	-2.825257	0.223067
48	2.763804	-1.308129	-1.994762
16	2.750086	1.338980	-2.350768
48	2.708926	2.495811	0.060676
16	2.401071	1.254073	2.417466
29	0.050002	1.109257	1.844835
16	0.085298	2.809930	0.095721
48	0.095101	1.163480	-2.003091
16	0.076974	-1.449549	-2.420403
48	0.042657	-2.406184	0.042757
16	0.176958	-1.217718	2.402088
48	-2.547220	-1.242936	2.208753
16	-2.575638	-2.843342	0.085122
48	-2.612301	-1.267431	-2.100583
16	-2.543189	1.390018	-2.402311
48	-2.560270	2.570215	0.004769
16	-2.343441	1.369150	2.370946
48	-5.004015	1.143576	1.949274
16	-5.259167	2.838140	0.078273
48	-5.126224	1.121794	-1.796563
16	-5.342561	-1.360312	-2.283960
48	-5.160398	-2.134658	0.122088
16	-5.265692	-1.311373	2.519594

****

4. **$Cd_{11}Cu_4S_{15}$ cluster:**

****

48	5.380057	1.768785	0.981320
16	5.261234	2.409315	-1.447483
29	5.468222	0.187920	-1.797525
16	5.453132	-2.068210	-1.755340
48	5.512533	-1.876691	0.757804
16	5.555974	-0.148251	2.597903
29	3.159197	-0.220520	2.321907
16	2.899063	-2.444019	1.261129
48	2.878004	-1.949787	-1.427275
16	2.015498	0.130134	-2.887026
48	2.673186	2.105720	-1.205257
16	2.711391	2.207516	1.514792
48	0.062827	1.984828	1.340262
16	0.028645	2.518166	-1.277981
29	-0.174665	0.263997	-2.247910
16	0.217840	-2.137865	-1.528499
48	0.279068	-1.966055	1.145939
16	0.940818	-0.035538	2.864404
29	-2.467786	-0.107360	1.689892
16	-2.303833	-2.334926	1.361177
48	-2.540184	-2.043685	-1.267928
16	-2.514465	0.190291	-2.671352
48	-2.702605	2.224798	-0.991152
16	-2.508282	2.150202	1.662076

48	-5.277303	1.555931	1.411610
16	-5.364074	2.382929	-1.020376
48	-5.151279	0.036670	-1.954913
16	-5.169847	-2.425484	-1.340575
48	-5.131455	-1.937860	1.180526
16	-6.019393	-0.327035	2.815310

****

5. **$Cd_{14}GaS_{15}$ cluster:**

****

48	5.365639	0.981140	-1.816057
16	5.466288	-1.543156	-2.099489
31	5.186914	-2.639410	0.006283
16	5.466234	-1.533156	2.106793
48	5.365638	0.989747	1.811405
16	5.530411	2.749651	-0.006506
48	2.824057	2.485364	-0.005864
16	2.772117	1.316948	2.418246
48	2.765850	-1.322571	2.142412
16	2.745671	-2.930240	0.007037
48	2.765954	-1.333128	-2.136460
16	2.772077	1.305280	-2.424238
48	0.127446	1.166377	-2.086570
16	0.082396	-1.476171	-2.421802
48	0.028612	-2.485287	0.005971
16	0.082353	-1.464250	2.428715

48	0.127414	1.176819	2.081394
16	0.148336	2.815850	-0.006800
48	-2.539924	2.543030	-0.006114
16	-2.510432	1.404167	2.420264
48	-2.619082	-1.248550	2.171488
16	-2.620846	-2.816807	0.006872
48	-2.619122	-1.259439	-2.165749
16	-2.510366	1.392178	-2.426770
48	-5.116048	1.151541	-1.886310
16	-5.348166	-1.322258	-2.399635
48	-5.202607	-2.115361	0.005120
16	-5.348178	-1.310348	2.405884
48	-5.116110	1.160921	1.880750
16	-5.250695	2.854357	-0.006995

****

6. **$Cd_{13}Ga_2S_{15}$ cluster:**

****

48	5.651592	2.870842	-0.177983
16	5.436562	1.247241	-2.360485
48	5.416259	-1.157297	-1.645484
16	5.583000	-2.610539	0.441650
48	5.358474	-0.677968	2.058176
16	4.979596	1.822140	2.373107
31	2.739640	1.418967	1.864717
16	2.706306	-0.909039	2.389225

48	2.849793	-2.534442	0.258786
16	2.789804	-1.709674	-2.238966
48	2.860866	1.003164	-2.161108
16	2.490659	2.750771	-0.082960
31	0.170554	2.250670	-0.016925
16	0.182064	1.115717	-2.090471
48	0.177221	-1.570020	-1.833870
16	0.140926	-2.936183	0.456567
48	0.026405	-0.993698	2.233415
16	0.410779	1.664601	2.278329
48	-3.045236	1.625221	1.819076
16	-2.573232	-0.889771	2.444733
48	-2.555825	-2.499042	0.264662
16	-2.407519	-1.568270	-2.218147
48	-2.586338	1.138269	-2.026963
16	-2.015029	2.982582	-0.110620
48	-6.265868	2.407002	-0.401682
16	-5.161725	1.125519	-2.478947
48	-5.058550	-1.302114	-1.817421
16	-5.225618	-2.852081	0.212941
48	-5.281646	-0.939223	1.872688
16	-5.616516	1.544984	2.077073

****

7. **$Cd_{11}Ga_4S_{15}$ cluster:**

****

48	-5.444208	0.380062	1.944120
16	-5.509940	-2.159846	1.677690
31	-6.155860	-2.443007	-0.564667
16	-5.451665	-1.105842	-2.230643
48	-5.708196	1.875029	-1.843264
16	-5.264693	2.647838	0.858407
31	-2.999279	2.102185	0.623707
16	-2.870938	1.643225	-1.686944
48	-2.834244	-0.982697	-2.021113
16	-2.042232	-3.113220	-0.678618
48	-2.748059	-1.995122	1.532976
16	-2.824633	0.471791	2.398504
48	-0.069160	0.953910	2.205777
16	0.063025	-1.665561	1.860374
31	0.080180	-2.176051	-0.475896
16	-0.055871	-0.598583	-2.250564
48	-0.184164	1.928672	-1.377027
16	-0.904429	3.062499	0.910919
31	2.991519	2.906667	0.713320
16	2.442812	2.152504	-1.506045
48	2.616707	-0.663548	-2.214756
16	2.267576	-2.838237	-0.705854
48	2.739303	-1.650003	1.628200
16	2.563391	1.161540	2.317231
48	5.253395	0.687990	2.015144

16 5.298825 -1.790791 1.951255

48 5.724348 -2.424833 -0.712304

16 5.147524 -0.604371 -2.721997

48 5.142245 1.617062 -1.617761

16 5.464013 2.802259 0.611909

****

8. **$Cd_{14}HgS_{15}$ cluster:**

****

48 -5.012505 1.326863 1.909935

16 -5.287491 -1.147466 2.480322

80 -5.319511 -1.843074 0.010528

16 -5.287613 -1.176225 -2.467224

48 -5.012449 1.304449 -1.924734

16 -5.149543 2.977055 -0.017077

48 -2.428044 2.652002 -0.015058

16 -2.419425 1.509087 -2.436824

48 -2.533638 -1.143096 -2.137280

16 -2.533969 -2.665465 0.015285

48 -2.533472 -1.117800 2.149470

16 -2.419448 1.537302 2.419981

48 0.230049 1.269778 2.078196

16 0.153430 -1.339441 2.470860

48 0.103927 -2.386157 0.013502

16 0.153411 -1.367932 -2.455943

48 0.230050 1.245127 -2.091628

16	0.262347	2.894649	-0.016614
48	2.957594	2.507185	-0.014250
16	2.878046	1.373836	-2.429288
48	2.834239	-1.293946	-2.167673
16	2.741037	-2.834582	0.016202
48	2.834077	-1.268345	2.181591
16	2.878104	1.401993	2.413913
48	5.459701	0.998469	1.874279
16	5.553110	-1.479502	2.411794
48	5.353774	-2.283385	0.013069
16	5.553267	-1.507383	-2.394879
48	5.459705	0.976579	-1.885345
16	5.693264	2.676277	-0.015368

****

9. **$Cd_{13}Hg_2S_{15}$ cluster:**

****

48	5.258127	-1.571251	1.188935
16	5.330098	0.360509	2.836425
48	5.098106	2.176114	1.084617
16	5.257511	2.650913	-1.405991
48	5.188366	0.223217	-2.147277
16	5.548021	-2.129822	-1.274053
80	2.726761	-2.076999	-1.190676
16	2.595042	0.110431	-2.837918
48	2.558562	2.313435	-1.297293

16 2.479252 2.606047 1.365027

48 2.600631 0.222216 2.557314

16 2.696910 -2.249087 1.540394

80 -0.060672 -1.961717 1.271074

16 -0.118691 0.182032 2.903286

48 -0.142805 2.205532 1.173226

16 -0.118122 2.498687 -1.469397

48 -0.061039 0.023236 -2.420431

16 -0.068476 -2.418566 -1.380324

48 -2.784727 -2.120354 -1.218852

16 -2.710646 -0.002861 -2.836178

48 -2.795026 2.215975 -1.343510

16 -2.781317 2.522682 1.318544

48 -2.837693 0.130187 2.496926

16 -2.808975 -2.309859 1.436717

48 -5.391766 -1.772902 1.069799

16 -5.580409 0.151522 2.717573

48 -5.376962 1.979438 0.975936

16 -5.506671 2.443899 -1.517151

48 -5.322561 0.019763 -2.252816

16 -5.517611 -2.356770 -1.398663

****

10. $Cd_{11}Hg_4S_{15}$ cluster:

****

48 -5.034307 1.230259 1.939084

16	-5.330214	-1.247988	2.478356
80	-5.392277	-1.896405	0.000037
16	-5.330219	-1.248084	-2.478308
48	-5.034306	1.230182	-1.939127
16	-5.263212	2.869743	-0.000054
80	-2.492772	2.640574	-0.000051
16	-2.452582	1.435367	-2.505205
48	-2.562871	-1.206908	-2.161679
16	-2.607251	-2.719295	0.000050
48	-2.562868	-1.206818	2.161717
16	-2.452582	1.435468	2.505152
48	0.212356	1.154197	2.104570
16	0.135376	-1.440592	2.538248
80	0.075591	-2.526224	0.000045
16	0.135377	-1.440689	-2.538200
48	0.212357	1.154111	-2.104606
16	0.241289	2.759068	-0.000053
80	3.003665	2.473349	-0.000047
16	2.880605	1.298618	-2.486323
48	2.823998	-1.367613	-2.187274
16	2.767925	-2.900634	0.000054
48	2.823994	-1.367521	2.187319
16	2.880604	1.298719	2.486275
48	5.457862	0.884835	1.898489
16	5.550985	-1.596109	2.412482

48	5.381503	-2.359086	0.000047
16	5.550991	-1.596203	-2.412418
48	5.457862	0.884760	-1.898516
16	5.795134	2.544946	-0.000047

****

11. $Cd_{14}InS_{15}$ cluster:

****

48	5.224397	1.179247	-1.829726
16	5.397726	-1.315678	-2.237624
49	5.303490	-2.561261	0.000287
16	5.397728	-1.315163	2.237908
48	5.224404	1.179673	1.829467
16	5.362556	2.927281	-0.000332
48	2.648832	2.615904	-0.000290
16	2.623315	1.457181	2.416597
48	2.699153	-1.190609	2.142186
16	2.693866	-2.793297	0.000323
48	2.699153	-1.191128	-2.141945
16	2.623309	1.456611	-2.416902
48	-0.014756	1.231549	-2.079013
16	0.018330	-1.405774	-2.426571
48	-0.001393	-2.436937	0.000273
16	0.018329	-1.405197	2.426869
48	-0.014754	1.232057	2.078765
16	-0.043389	2.879924	-0.000331

48	-2.721599	2.525593	-0.000285
16	-2.659170	1.383089	2.423018
48	-2.683672	-1.272584	2.167938
16	-2.639626	-2.837317	0.000327
48	-2.683678	-1.273115	-2.167675
16	-2.659166	1.382511	-2.423313
48	-5.253362	1.058604	-1.882800
16	-5.409670	-1.419977	-2.403075
48	-5.240479	-2.211620	0.000255
16	-5.409667	-1.419407	2.403394
48	-5.253366	1.059055	1.882567
16	-5.443052	2.752007	-0.000319

****

12. $Cd_{13}In_2S_{15}$ cluster:

****

48	4.247741	-2.424842	-0.201653
16	4.948604	-1.589894	2.203293
48	4.408454	0.891036	2.102111
16	4.994193	2.543437	0.121479
48	4.354906	1.241730	-1.930854
16	4.762554	-1.317544	-2.386381
49	2.544390	-1.137769	-3.685198
16	2.526397	1.428073	-3.738049
48	2.728258	3.473222	0.912141
16	2.595234	2.319719	3.240843

48	2.619475	-2.487974	2.683470
16	2.297595	-4.008055	0.526135
49	0.341701	-2.558119	0.106694
16	0.370427	-1.326596	2.367982
48	0.374673	1.371634	2.296316
16	0.406435	2.974885	-0.022685
48	0.440071	1.513980	-2.199769
16	0.535667	-1.284455	-2.026210
48	-2.396156	-1.199162	-1.985987
16	-2.168782	1.415387	-2.367599
48	-2.300057	2.572807	0.017557
16	-2.236246	1.361867	2.374849
48	-2.548948	-1.249369	2.019793
16	-2.074913	-2.904302	0.018912
48	-5.659672	-2.399559	-0.066506
16	-5.149572	-1.244363	2.299732
48	-4.956034	1.218567	1.847373
16	-4.962792	2.942580	-0.024768
48	-4.874646	1.226326	-1.909950
16	-4.997650	-1.237272	-2.380496

****

13. $Cd_{11}In_4S_{15}$ cluster:

****

48	5.707379	1.771422	-1.960669
16	5.319902	-1.095990	-2.250484

49	5.296342	-2.762937	-0.426748
16	5.342348	-1.951423	2.020064
48	5.336868	0.575040	1.934256
16	5.305327	2.760372	0.685724
49	2.849918	2.389453	0.489576
16	2.679497	0.845861	2.528331
48	2.670145	-1.721398	1.953627
16	2.401627	-2.915041	-0.395239
48	2.770385	-0.797460	-2.154741
16	2.714401	1.844481	-1.953564
48	0.054071	1.858277	-1.632331
16	0.056943	-0.768814	-2.354611
49	-0.015683	-2.283680	-0.352251
16	-0.073587	-1.633321	2.091129
48	-0.035574	1.049539	2.214479
16	0.481861	3.121990	0.679720
49	-3.065829	2.959900	0.528990
16	-2.678967	1.136956	2.304915
48	-2.795879	-1.615642	1.765186
16	-2.372386	-2.903333	-0.538854
48	-2.670490	-0.836901	-2.224917
16	-2.576499	1.941066	-1.785145
48	-5.292357	1.343982	-1.738879
16	-5.210933	-0.940207	-2.706220
48	-5.639127	-2.669060	-0.588413

16 -5.359859 -1.834511 2.037044

48 -5.386854 0.645197 1.932408

16 -5.696166 2.655798 0.403497

****