Supporting Information

for

Structure Predictions for Nanoscale Magic-Sized CdSe Clusters from a New Efficient Structure-Searching Strategy

Gaolu Zhang,[a] Xin Wang *[a] and Dingguo Xu *[a]

[a]MOE Key Laboratory of Green Chemistry and Technology, College of Chemistry, Sichuan University, Chengdu, Sichuan, 610064, PR China

* To whom correspondence should be addressed: wangxin@scu.edu.cn (X.W) dgxu@scu.edu.cn (D.X), Tel: 86-28-85406156.

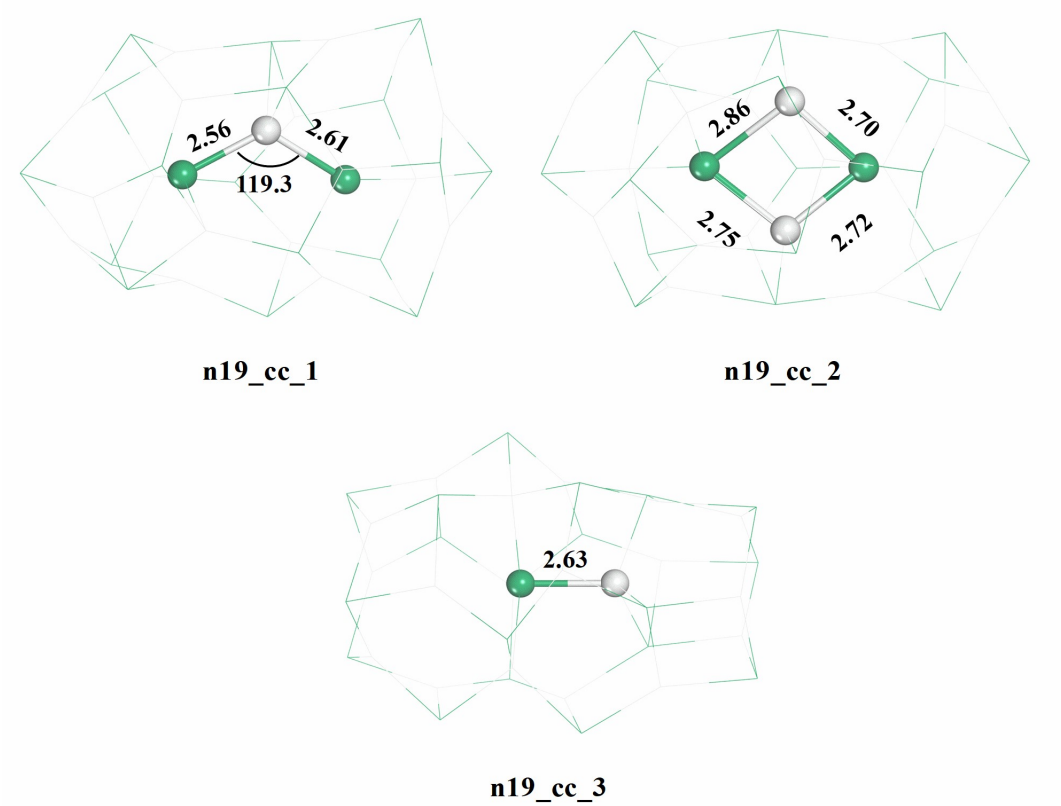


Fig. S1 Core structure and bond lengths of the core@cage structures in $(CdSe)_{19}$ MSCs. Cadmium and selenium atoms are in silver and green colors, respectively. Bond lengths and angle are in angstrom and degree, respectively.

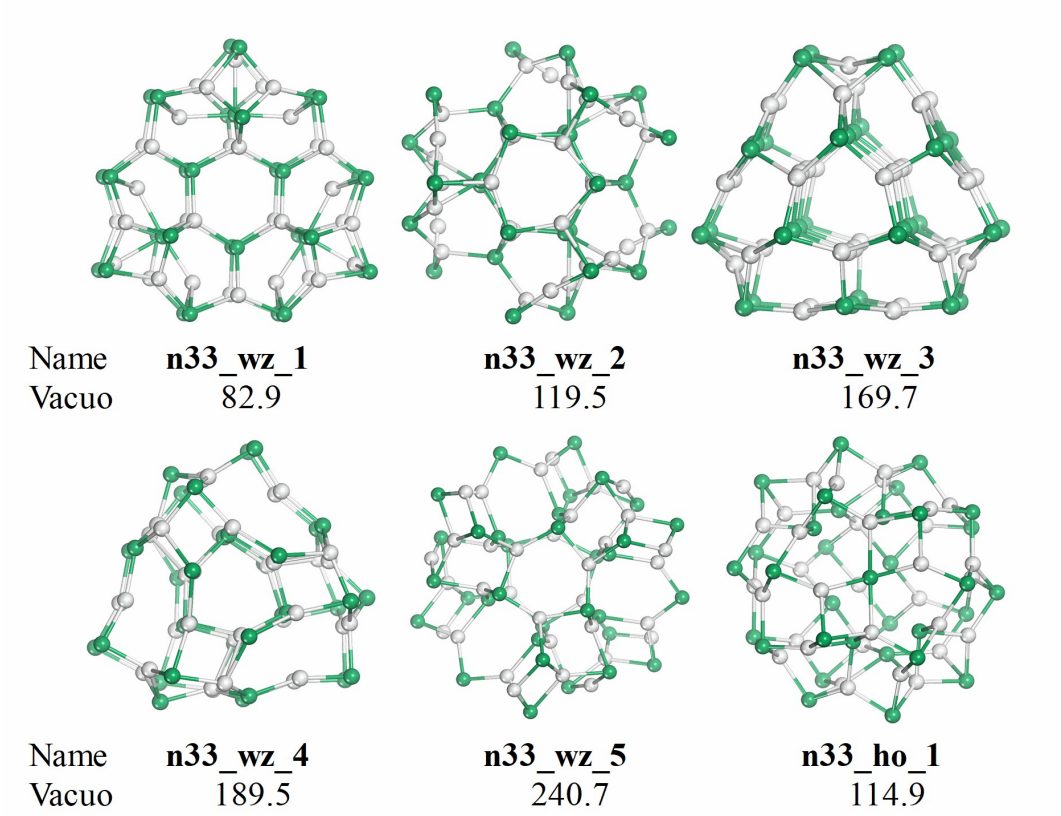


Fig. S2 PBE optimized structures of the identified wurtzite-like and hollow isomers from the extended search of the 500 lowest-energy structures for $(CdSe)_{33}$. The relative energies, referenced to that of the lowest-energy structure **n33_$(CdSe)_6$@$(CdSe)_{27}$_1** in vacuo, are given in kcal/mol. The colour settings are the same as Fig. S1.

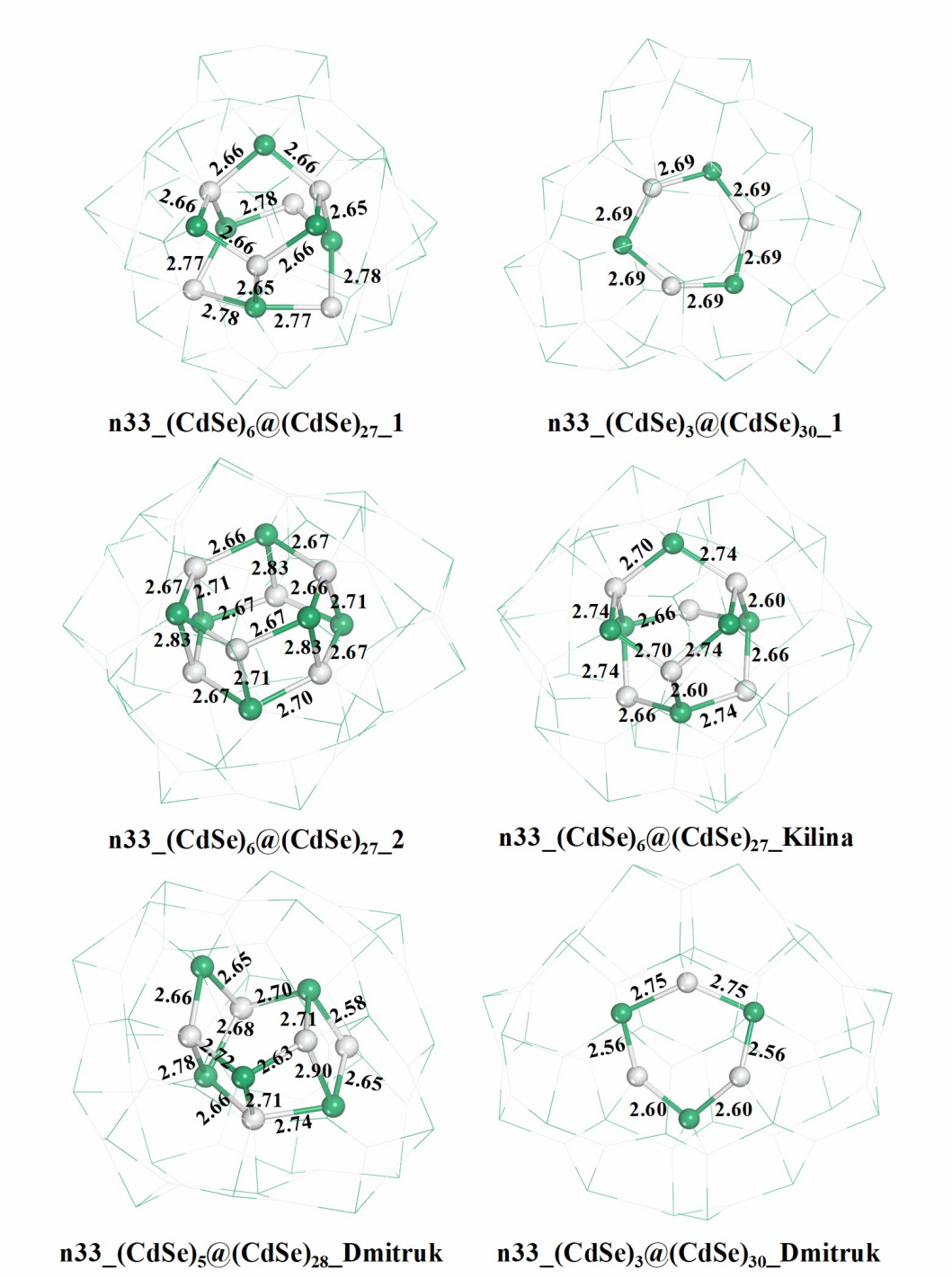
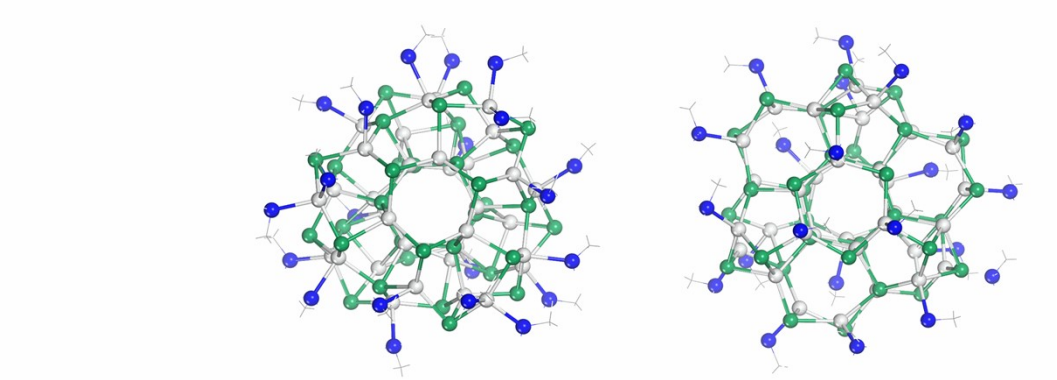


Fig. S3 Core structure and bond lengths of the core@cage structures in $(CdSe)_{33}$ MSCs. The colour settings are the same as Fig. S1. Bond lengths are in angstrom.



Name	**n33_$(CdSe)_6$@$(CdSe)_{27}$_1**	**n33_$(CdSe)_6$@$(CdSe)_{27}$_Kilina**
$(CdSe)_{33}$	0.0	39.0
$(CdSe)_{33}(MeNH_2)_{21}$	0.0	17.2

Fig. S4 PBE optimized structures of ligand-passivated **n33_$(CdSe)_6$@$(CdSe)_{27}$_1** and **n33_$(CdSe)_6$@$(CdSe)_{27}$_Kilina** with 21 methylamine ($MeNH_2$) ligands. The relative energies of bare and ligand-passivated $(CdSe)_{33}$ isomers are given in kcal/mol. Cadmium, selenium, nitrogen atoms are in silver, green and blue colors, respectively. The carbon and hydrogen atoms are in lines.

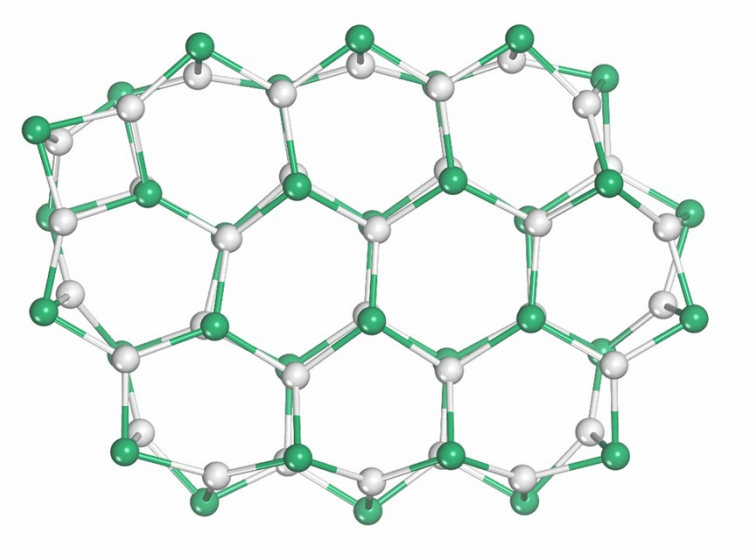


Fig. S5 A wurtzite-like cage $(CdSe)_{33}$ structure. The colour settings are the same as Fig. S1.

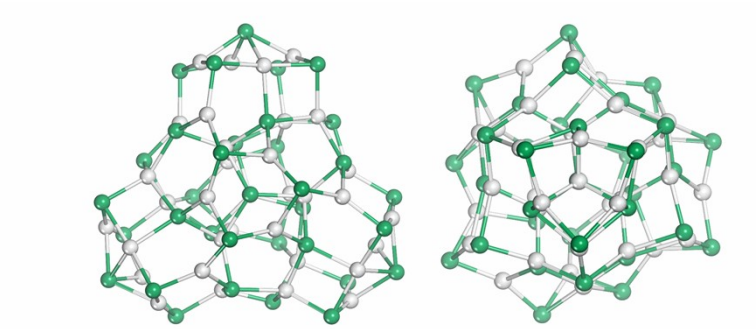


Fig. S6 PBE optimized structures of the identified wurtzite-like isomers from the extended search of the 500 lowest-energy structures for $(CdSe)_{34}$. The relative energies, referenced to that of the lowest-energy structure **n34_Cd_4Se_6@$Cd_{30}Se_{28}$_1** in vacuo, are given in kcal/mol. The colour settings are the same as Fig. S1.

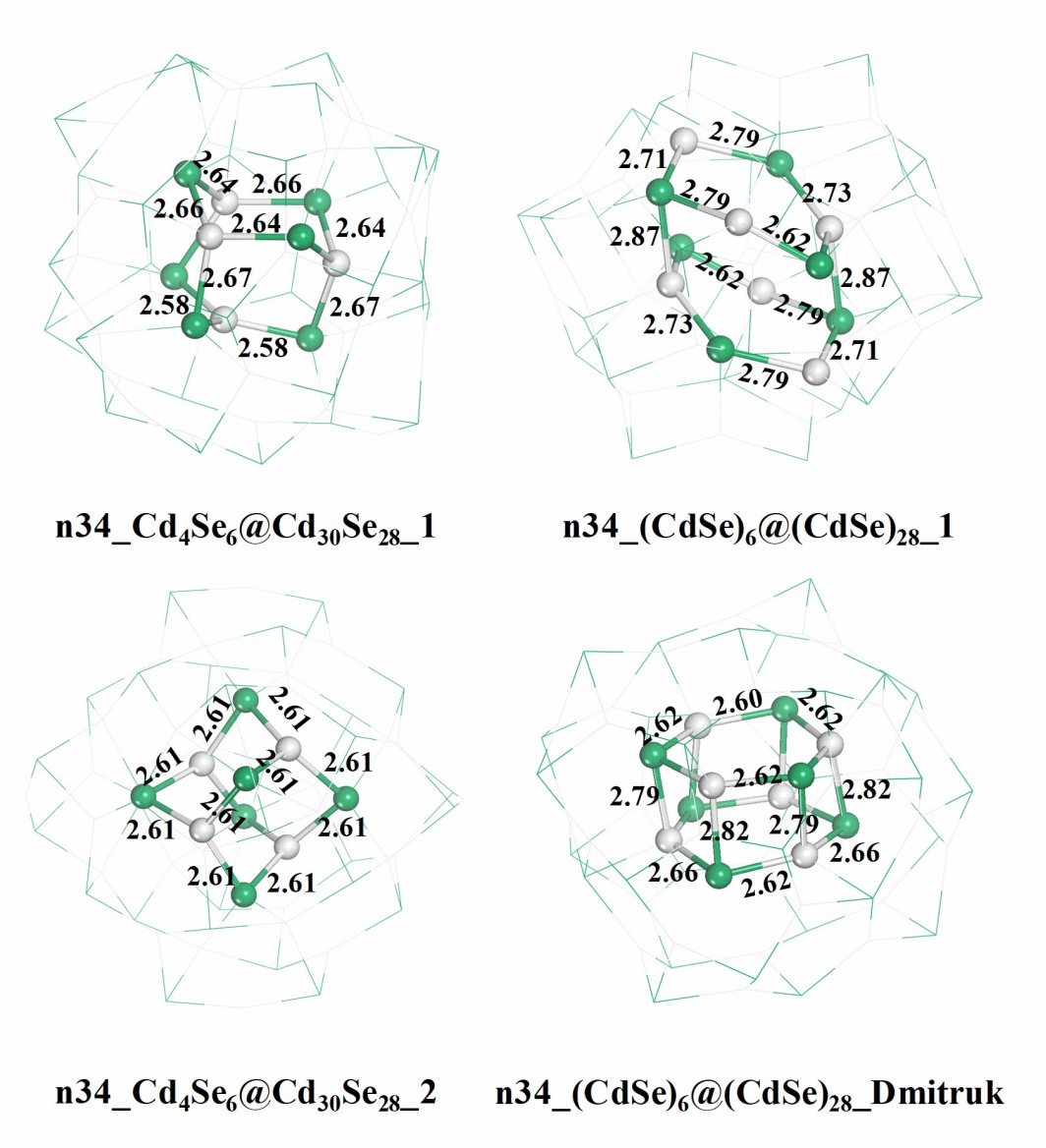


Fig. S7 Core structure and bond lengths of the core@cage structures in $(CdSe)_{34}$ MSCs. The colour settings are the same as Fig. S1. Bond lengths are in angstrom.

To verify the structural stability of the core@cage configurations at ambient conditions, we conducted 7 ps ab initio molecular dynamics (AIMD) calculations (with a 1 fs time step) using **n33_$(CdSe)_6$@$(CdSe)_{27}$_1** and **n34_Cd_4Se_6@$Cd_{30}Se_{28}$_1** at 298.15 K in an implicit toluene solvent model. The calculations were performed using the CP2K program with the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional and D3(BJ) dispersion corrections. Core electrons were modeled using Goedecker-Teter-Hutter (GTH) pseudopotentials, with energy cutoffs set to 45 Ry for the wave function and 450 Ry for electronic density. The DZVP-MOLOPT-SR-GTH basis set (a double-zeta Gaussian with polarization) was employed with a convergence criterion of 1.0×10^{-6}. Solvent effects were incorporated using the self-consistent reaction field (SCRF) model. The structural evolution over time, illustrated in Fig. S8, confirms that the core@cage structures remain intact throughout the simulation.

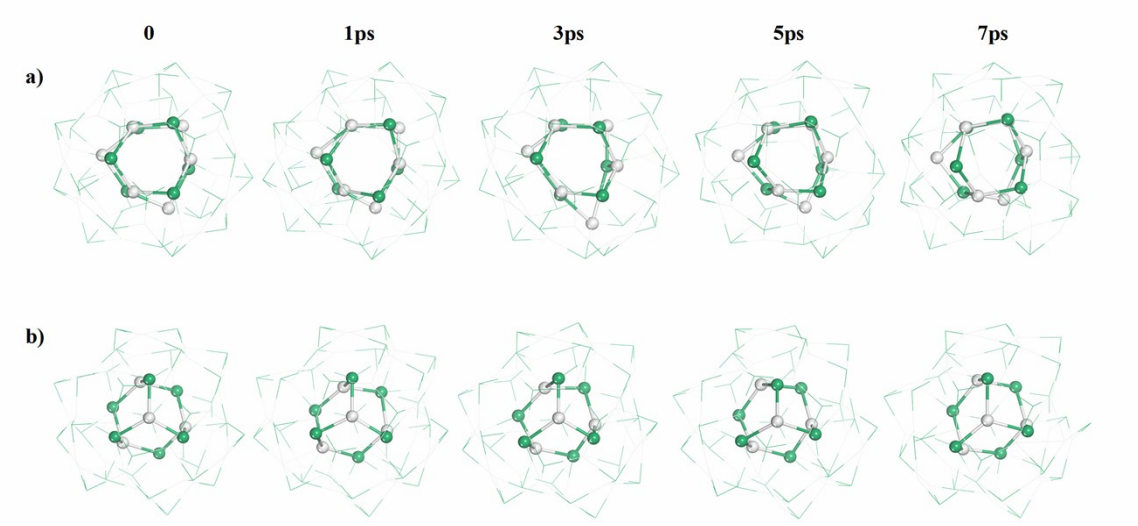


Fig. S8 Screenshots of AIMD calculations for a) **n33_$(CdSe)_6$@$(CdSe)_{27}$_1** and b) **n34_Cd_4Se_6@$Cd_{30}Se_{28}$_1** at 298.15 K in an implicit toluene solvent environment. The colour settings are the same as Fig. S1.

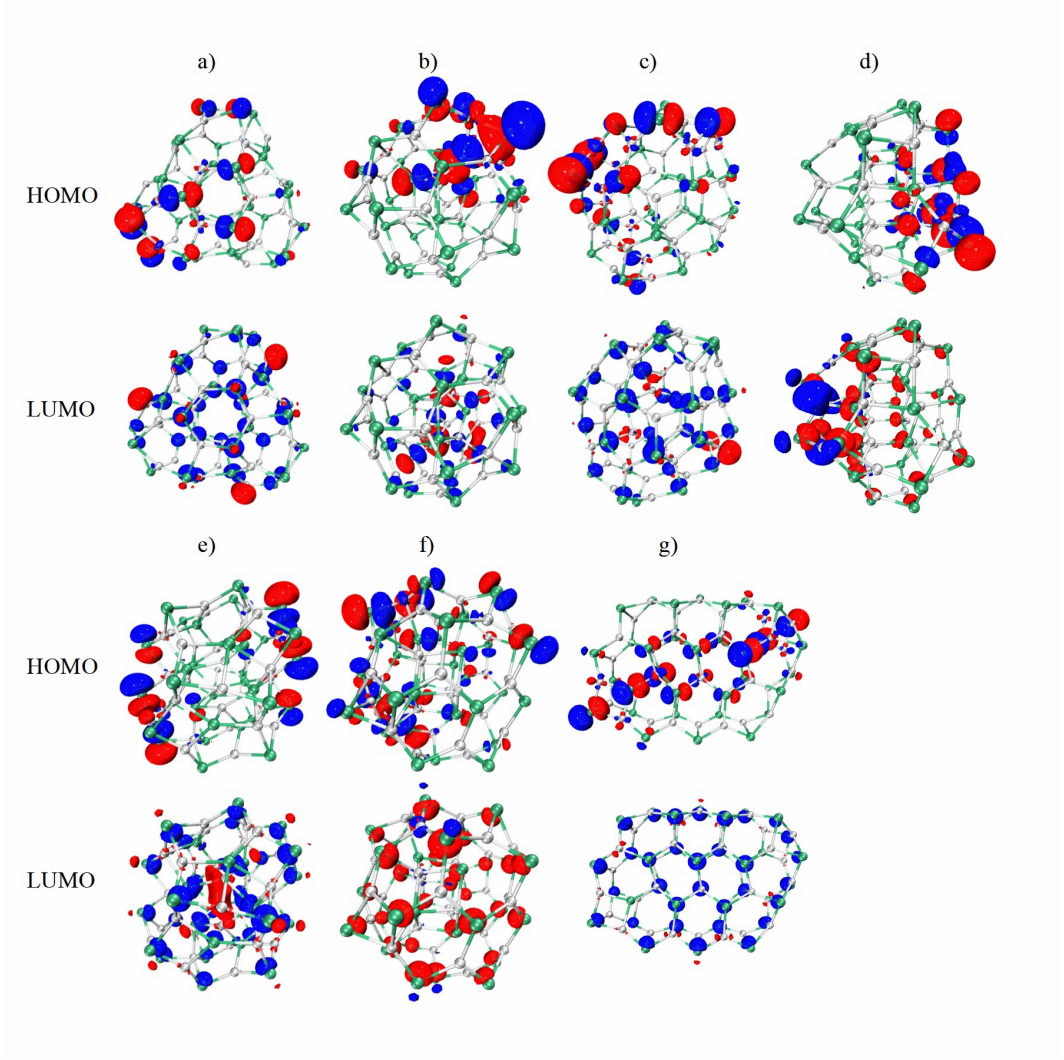


Fig. S9 Spatial configuration of HOMO and LUMO calculated for $(CdSe)_{33}$ and $(CdSe)_{34}$ MSCs isomers: a) **n33_$(CdSe)_3$@$(CdSe)_{30}$_1**; b) **n33_$(CdSe)_5$@$(CdSe)_{28}$_Dmitruk**;c) **n33_$(CdSe)_3$@$(CdSe)_{30}$_Dmitruk**; d) **n33_$(CdSe)_6$@$(CdSe)_{27}$_Kilina**; e) **n34_$(CdSe)_6$@$(CdSe)_{28}$_1**; f) **n34_$(CdSe)_6$@$(CdSe)_{28}$_Dmitruk**; g) **n34_wz_1**. Red represents the positive phase of the orbital wave function, while blue represents the negative phase.

Inverse participation ratio (IPR) is an index used to quantitatively characterize the localization degree of a wave function.[1-5] If the KS states are expressed as a linear combination of atom-centered basis functions, i.e., $\Psi_n(r) = \sum_i^N c_{ni}\Phi_i(r)$ where Φ_i are the basis functions, the IPR is defined as:

$$IPR(\Psi_n) = \frac{\sum_i^N c_{ni}^4}{(\sum_i^N c_{ni}^2)^2}, \qquad (1)$$

A larger IPR value indicates a higher concentration of the wave function within a finite local region, suggesting a more localized electronic state. Conversely, a smaller IPR value signifies a more dispersed wave function across multiple basis functions, implying a more extended electronic state. In a fully extended state, all N basis functions contribute equally, resulting in an IPR of approximately 1/N. Conversely, for localized states, the IPR approaches 1.

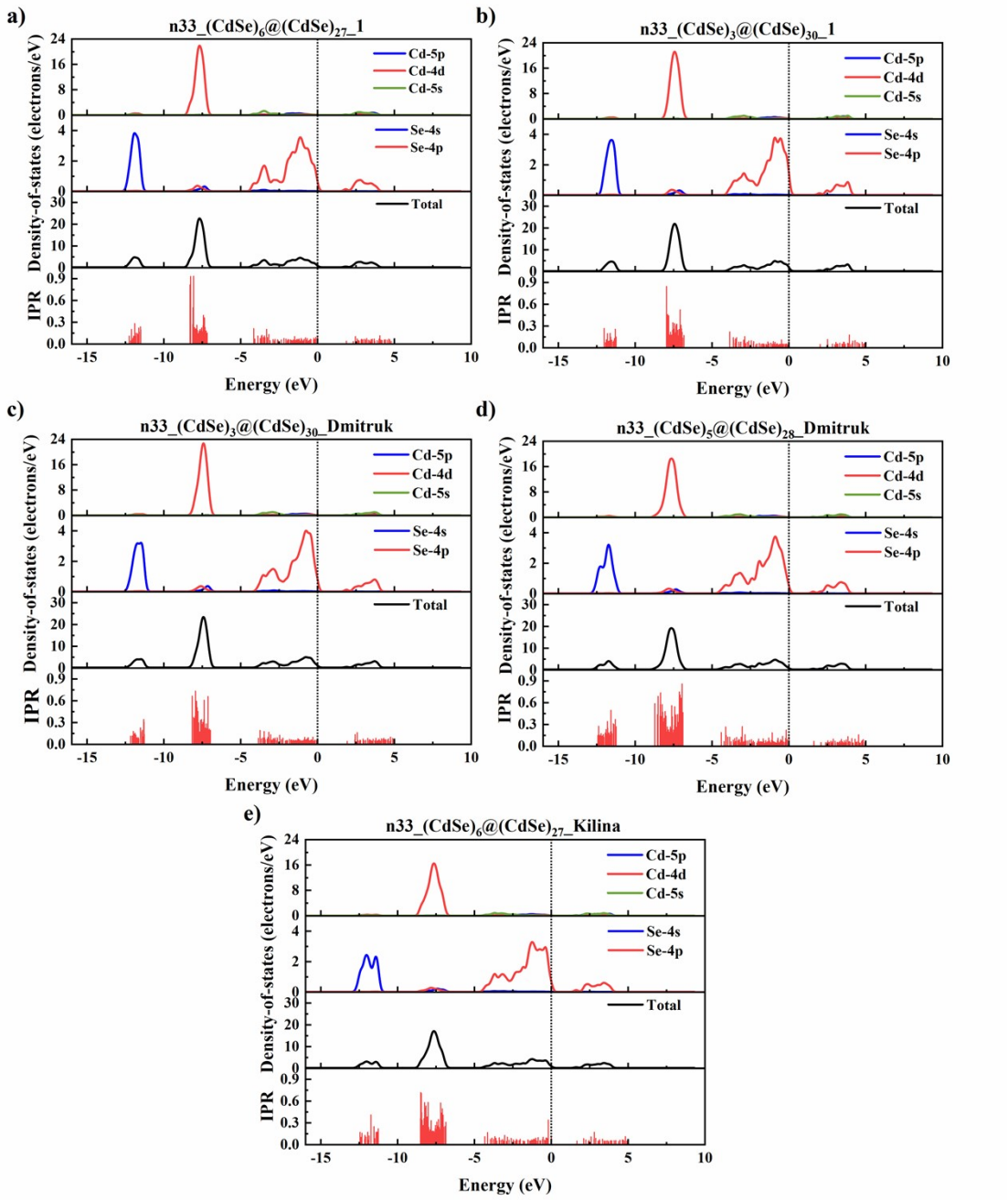


Fig. S10 Inverse participation ratio (IPR) spectrum and density of states (DOS) of $(CdSe)_{33}$ MSCs isomers, along with the projected density of states (PDOS) on Cd and Se orbitals.

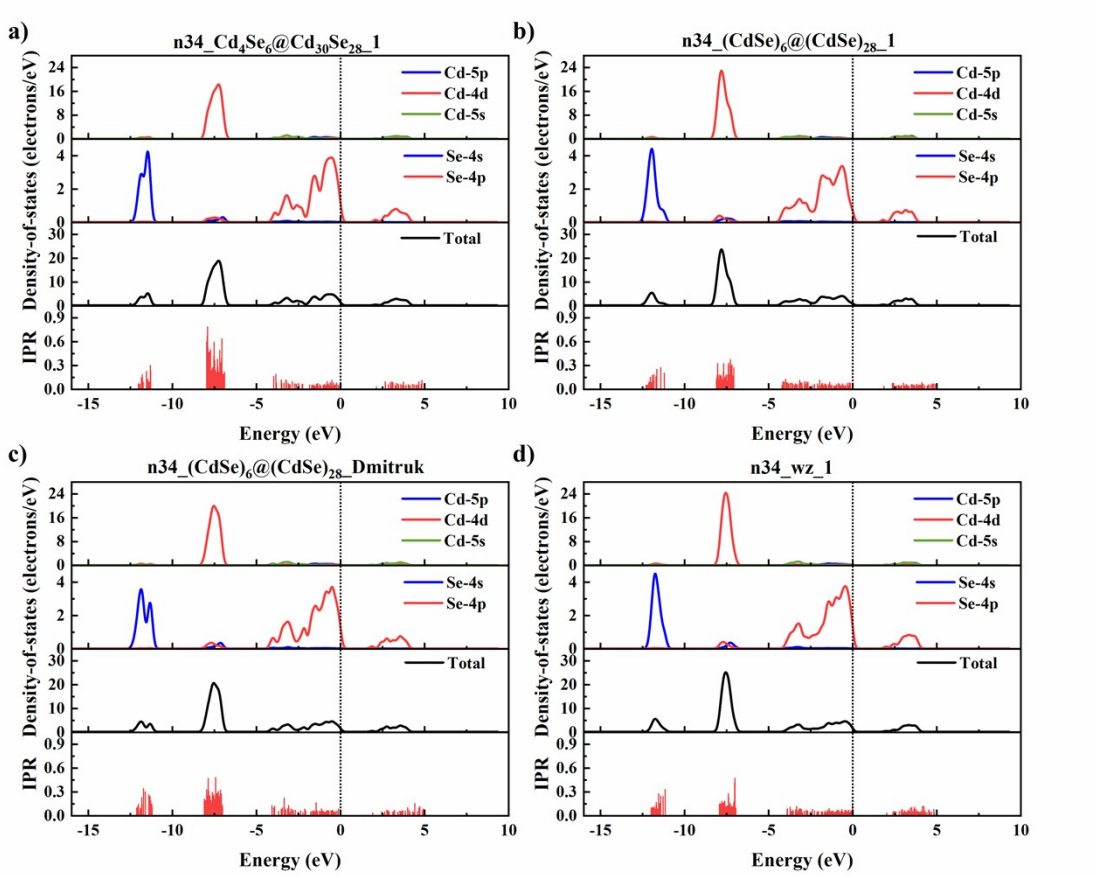


Fig. S11 Inverse participation ratio (IPR) spectrum and density of states (DOS) of $(CdSe)_{34}$ MSCs isomers, along with the projected density of states (PDOS) on Cd and Se orbitals.

Table S1 Average Cd-Se bond lengths (Å), angles (°), and average absolute (abs) dihedral angles (°) of $Cd_{14}Se_{13}^{2+}$ structure, which was optimized by GFN1-xTB and CP2K for comparison with experimental values.[6] Average Cd-Se core bond lengths and angles were also listed.

methods	bond lengths	bond angles	abs dihedral angles	core bond lengths	core bond angles
Exp[6]	2.61	105.8	81.4	2.7	107.5
GFN1-TB	2.62	104.6	84.6	3.1	101.3
CP2K	2.66	104.6	83.3	2.8	107.2

Table S2 Optimization time using different methods for $(CdSe)_{19}$ cluster and corresponding hardware configurations.[a]

methods	time/N[b]	time/N	time/N
XTB	—	—	57h/10000
PBE	110h/50	660h/300	22000h/10000[c]
XTB+PBE	—	—	167h/(10000+50)[d]

[a] CPU: Intel(R) Xeon(R) Gold 6230 CPU @ 2.10GHz; Cores: 40; Memory: 128G. [b] N is the numbers of $(CdSe)_n$ structures. [c] estimated time for 10000 structures. [d] total calculation time for 10000 and 50 structures by XTB and PBE methods, respectively.

Table S3 Coordinates of atoms in optimized structure of **n13_cc_1**.

Particle Type	Coordinates (Angstroms)		
	X	Y	Z
Cd	11.66235	11.97961	9.22049
Cd	6.66062	11.20259	11.03072
Cd	10.53914	7.33323	9.18282
Cd	8.98167	13.41644	11.16501
Cd	7.39399	7.51205	11.4849
Cd	12.61871	9.271	11.37716
Cd	8.32996	12.0041	7.70556
Cd	7.13712	8.46429	8.42895
Cd	13.18526	9.19958	8.0094
Cd	9.5051	10.01385	13.00472
Cd	10.58972	6.77966	12.53327
Cd	11.91756	12.37253	12.63141
Cd	10.14578	9.66932	6.45755
Se	6.99456	13.35184	9.44761
Se	8.1985	6.17259	9.32649
Se	14.10447	10.7796	9.71529
Se	12.52879	6.61272	10.96391
Se	11.49489	14.13371	10.89619
Se	5.46944	8.98761	10.47428
Se	7.53016	9.85545	6.29695
Se	11.73455	7.59583	6.73795
Se	10.82495	12.2297	6.75374
Se	7.92583	12.08889	13.22052
Se	8.58989	7.57193	13.82368
Se	12.13034	10.20273	13.85492
Se	9.96672	9.92295	10.20263

Table S4 Coordinates of atoms in optimized structure of **n13_ho_1**.

Particle Type	Coordinates (Angstroms)		
	X	Y	Z
Cd	11.05443	8.56918	8.38435
Cd	7.20296	8.1174	7.56591
Cd	8.81988	9.36168	13.73875
Cd	12.99308	9.47849	14.05151
Cd	7.76493	7.41157	11.20247
Cd	11.5221	12.07029	12.83451
Cd	10.97599	11.79969	9.06504
Cd	7.30103	11.82106	7.5247
Cd	13.69478	9.79782	10.89389
Cd	9.2394	9.88116	5.82047
Cd	5.90743	10.0345	10.58759
Cd	11.03659	7.51465	12.14956
Cd	8.03897	12.3077	11.38107
Se	10.78555	10.59746	14.94969
Se	13.07636	10.22464	8.43009
Se	6.54913	9.94794	5.79032
Se	6.70929	10.74232	13.0667
Se	5.71634	7.57041	9.65842
Se	8.89888	6.66323	13.39629
Se	13.57873	7.50665	12.36568
Se	9.62973	7.36777	6.61064
Se	9.79776	12.27463	6.73806
Se	5.99526	12.47784	9.63077
Se	10.32833	13.47402	11.02143
Se	14.13246	11.5602	12.80103
Se	9.69031	9.32479	10.56779

Table S5 Coordinates of atoms in optimized structure of **n13_wz_1**.

Particle Type	Coordinates (Angstroms)		
	X	Y	Z
Cd	5.94727	11.76327	9.13942
Cd	9.92631	6.35262	9.1389
Cd	12.62381	12.50441	9.13874
Cd	10.47654	12.61327	11.92711
Cd	6.92708	9.85025	11.92731
Cd	11.09354	8.15796	11.92669
Cd	14.06755	10.8398	11.46594
Cd	6.66553	13.84703	11.46605
Cd	7.76352	5.93297	11.46631
Cd	8.86038	14.03098	9.13865
Cd	6.50629	7.74108	9.13868
Cd	13.13115	8.84709	9.13801
Cd	9.49874	10.20667	8.52985
Se	13.67771	8.28124	11.74927
Se	9.07639	14.78852	11.74954
Se	5.74283	7.55022	11.7498
Se	10.46793	12.59199	7.70949
Se	6.94864	9.85279	7.70946
Se	11.08041	8.1752	7.70934
Se	5.16101	11.74076	11.75051
Se	10.33973	5.68312	11.75011
Se	12.99695	13.1964	11.75004
Se	14.69797	10.92826	8.80127
Se	6.27469	14.34762	8.80123
Se	7.52466	5.34346	8.80151
Se	9.49906	10.20736	11.38806

Table S6 Coordinates of atoms in optimized structure of **n19_cc_1**.

Particle Type	Coordinates (Angstroms)		
	X	Y	Z
Cd	12.44672	10.39789	13.4248
Cd	8.08545	11.41617	13.36528
Cd	6.07142	6.30804	11.11966
Cd	12.65712	7.54214	10.56372
Cd	13.73025	13.32498	11.93282
Cd	6.7956	11.74799	9.82961
Cd	5.59512	9.56792	12.71585
Cd	15.11026	10.41359	10.91145
Cd	12.94219	10.89191	5.6408
Cd	7.4944	8.9753	7.63247
Cd	8.72076	7.66811	13.11222
Cd	10.35982	10.03436	11.21674
Cd	13.56711	12.91584	8.38833
Cd	10.09308	11.80038	7.42103
Cd	8.87167	6.53597	9.67783
Cd	11.38422	8.37111	7.36985
Cd	4.80421	8.65146	9.31816
Cd	14.89246	9.23991	8.02082
Cd	10.57315	13.31322	10.48925
Se	9.47695	9.62409	6.0671
Se	12.12629	13.19581	6.15983
Se	5.8381	12.18988	12.25913
Se	14.80265	11.51468	13.33547
Se	11.50344	8.04169	12.96291
Se	7.40518	9.23381	14.70477
Se	11.29266	6.18947	8.79093
Se	8.27278	5.32309	12.05102
Se	3.98123	7.78706	11.64155
Se	15.24051	7.86573	10.28819
Se	12.1179	10.54724	9.36094
Se	8.04393	9.18585	10.54683
Se	12.769	14.80712	10.17723
Se	8.61345	13.43089	8.84245
Se	5.39116	10.65301	7.83023
Se	15.86866	11.67257	8.68481
Se	13.68387	8.50225	5.82494
Se	6.47538	6.5112	8.32161
Se	10.54745	12.31614	13.01556

Table S7 Coordinates of atoms in optimized structure of **n19_ho_1**.

Particle Type	Coordinates (Angstroms)		
	X	Y	Z
Cd	9.31804	13.90229	13.68422
Cd	9.31949	6.1406	6.37517
Cd	10.79651	6.7739	12.61123
Cd	10.80218	13.26452	7.44409
Cd	7.29112	12.18747	7.41153
Cd	7.2888	7.85616	12.64847
Cd	6.49904	8.09615	7.27374
Cd	6.49455	11.94953	12.78539
Cd	8.34395	14.09799	10.42893
Cd	8.34303	5.94744	9.62947
Cd	9.02014	10.19436	14.79368
Cd	9.03154	9.85373	5.26843
Cd	12.87371	9.28334	12.19425
Cd	12.89314	10.76602	7.85543
Cd	12.03004	11.53322	14.38618
Cd	12.03672	8.51115	5.67211
Cd	12.2187	7.36977	9.19311
Cd	12.22224	12.68025	10.862
Cd	8.5977	10.02422	10.02861
Se	8.5169	14.44684	7.6659
Se	8.50977	5.59402	12.39215
Se	11.14476	8.74466	14.48431
Se	11.15913	11.30145	5.56607
Se	10.05903	7.57468	4.31828
Se	10.05459	12.46997	15.74347
Se	10.67059	5.38679	8.4755
Se	10.67013	14.65819	11.58487
Se	13.92476	11.63227	12.67868
Se	13.93132	8.41094	7.37991
Se	6.51662	10.27469	5.83202
Se	6.5068	9.76942	14.22488
Se	13.21773	13.26961	8.45098
Se	13.21129	6.77894	11.60554
Se	6.78384	8.13483	9.99293
Se	6.7821	11.91256	10.06605
Se	6.87336	14.48213	12.90366
Se	6.87384	5.56294	7.15518
Se	11.14138	10.02536	10.02067

Table S8 Coordinates of atoms in optimized structure of **n19_wz_1**.

Particle Type	Coordinates (Angstroms)		
	X	Y	Z
Cd	7.38648	7.15715	12.52757
Cd	11.05396	7.44192	7.1927
Cd	8.56212	13.14344	9.52334
Cd	7.26284	11.76181	12.60353
Cd	12.14244	11.59404	8.68524
Cd	8.50068	5.69304	9.39284
Cd	4.80305	7.58916	10.21751
Cd	14.55989	8.61701	7.99583
Cd	11.80115	14.9621	9.59032
Cd	7.78807	9.49116	9.23927
Cd	15.65618	10.95142	10.2488
Cd	12.58936	5.10074	8.49876
Cd	11.16282	5.57125	11.96649
Cd	14.57156	13.89799	11.71054
Cd	4.78418	11.39845	10.23625
Cd	10.95659	13.38235	12.23379
Cd	14.14558	7.1225	11.37152
Cd	4.09162	9.46582	12.71944
Cd	11.09342	9.29101	11.39758
Se	16.75434	12.76571	11.69318
Se	6.6322	11.77523	8.44885
Se	13.35971	4.56726	10.87754
Se	16.06649	8.29855	10.16195
Se	2.98028	9.49204	10.22173
Se	12.62174	15.62297	11.87625
Se	4.81896	6.96007	12.86508
Se	12.23001	7.70121	13.1049
Se	8.47919	14.02514	12.03606
Se	4.71543	12.00443	12.90101
Se	12.56581	11.55571	11.4478
Se	8.64197	4.95238	11.90885
Se	8.43338	9.51392	11.96994
Se	10.09674	4.99911	7.47417
Se	14.54542	11.24642	7.77068
Se	6.61832	7.25839	8.41331
Se	10.56217	13.68798	7.83993
Se	13.51539	6.73051	6.57411
Se	10.45008	9.45371	8.7142

Table S9 Coordinates of atoms in optimized structure of **n33_(CdSe)$_6$@(CdSe)$_{27}$_1**.

Particle Type	Coordinates (Angstroms)		
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Cd	18.83598	10.8822	15.00716
Cd	18.8373	17.12447	18.39001
Cd	18.83759	16.93153	11.291
Cd	10.63984	11.34518	10.68309
Cd	10.64029	13.15038	20.1451
Cd	10.63904	20.43931	13.85491
Cd	13.8695	15.76234	12.69294
Cd	13.87047	12.68071	15.3164
Cd	13.87105	16.49445	16.67468
Cd	16.42872	15.83926	20.00453
Cd	16.42799	18.9715	11.59618
Cd	16.42988	10.12416	13.08305
Cd	11.25624	14.74113	10.66066
Cd	11.25719	11.43135	17.21695
Cd	11.25727	18.76577	16.80794
Cd	16.99113	13.44467	12.30993
Cd	16.99124	13.50836	17.51713
Cd	16.99094	17.98509	14.85778
Cd	14.01419	12.2557	10.58837
Cd	14.01442	12.6127	19.40544
Cd	14.01389	20.06898	14.68812
Cd	12.5782	18.81889	11.50555
Cd	12.57985	10.1235	13.26155
Cd	12.57969	15.99349	19.91534
Cd	20.18462	14.38084	17.05165
Cd	20.1841	17.1451	14.33763
Cd	20.18424	13.41299	13.30207
Cd	10.07323	16.93397	13.71073
Cd	10.07294	12.97316	13.79266
Cd	10.07347	15.02842	17.18157
Cd	15.68673	18.88269	18.2662
Cd	15.68568	15.94806	9.8283
Cd	15.68562	10.10856	16.58791
Se	18.81003	19.11391	13.16652
Se	18.81038	11.41577	12.17847
Se	18.8095	14.4083	19.34176
Se	11.8389	12.72992	8.98899
Se	11.83916	10.9904	19.79473

Se	11.83919	21.21784	15.89922
Se	17.358	17.90746	9.34438
Se	17.35698	8.70806	15.13308
Se	17.3567	18.32219	20.20736
Se	9.19246	14.93693	12.22795
Se	9.19312	12.69075	16.26428
Se	9.19307	17.31093	16.19324
Se	16.20838	20.19303	16.09502
Se	16.20871	13.41267	9.77913
Se	16.20857	11.33203	18.80905
Se	14.43287	20.55804	12.07546
Se	14.43402	9.74794	11.47007
Se	14.43342	14.62964	21.1369
Se	12.81983	13.32955	12.96649
Se	12.82029	14.13443	17.28617
Se	12.81978	17.47241	14.43107
Se	13.07394	18.27981	18.6947
Se	13.07259	16.61839	10.1364
Se	13.07294	10.03871	15.85239
Se	16.4855	12.67191	14.92756
Se	16.48597	16.16179	16.87814
Se	16.48416	16.10563	12.87955
Se	20.92138	16.91497	16.80017
Se	20.9211	15.65985	12.26894
Se	20.92068	12.36245	15.6218
Se	9.95907	19.0475	11.90265
Se	9.96023	10.35131	12.86527
Se	9.96017	15.53693	19.9159

Table S10 Coordinates of atoms in optimized structure of **n33_(CdSe)$_3$@(CdSe)$_{30}$_1**.

Particle Type	Coordinates (Angstroms)		
	X	Y	Z
Cd	14.33502	17.93771	17.46196
Cd	18.03748	17.93773	15.57667
Cd	14.55326	17.93904	13.3122
Cd	11.10798	17.51544	15.58463
Cd	18.02669	17.5168	19.30977
Cd	17.79129	17.51625	11.45518
Cd	21.43369	13.27795	17.13939
Cd	14.21503	13.27739	9.59017
Cd	11.28694	13.2763	19.61342
Cd	17.52724	14.46021	13.9423
Cd	13.39544	14.46008	14.57033
Cd	16.00548	14.46072	17.83645
Cd	17.98341	11.73004	9.74
Cd	9.53075	11.72857	16.27675
Cd	19.41916	11.72995	20.3272
Cd	21.28583	17.19829	17.65969
Cd	14.73782	17.19867	9.45695
Cd	10.90607	17.19639	19.22937
Cd	18.06876	12.21972	16.7117
Cd	15.52482	12.21963	12.7159
Cd	13.33797	12.21771	16.91674
Cd	12.10096	15.6719	11.34604
Cd	13.86158	15.67135	20.57036
Cd	20.96686	15.67324	14.42984
Cd	20.18242	12.13619	13.23304
Cd	11.45493	12.13531	12.62467
Cd	15.29372	12.13545	20.48985
Cd	8.92741	13.90631	14.19211
Cd	17.91629	13.90756	21.89306
Cd	20.09068	13.90746	10.25994
Cd	21.18923	15.33882	20.39398
Cd	17.15557	15.33888	8.17416
Cd	8.58741	15.33665	17.77637
Se	15.5426	11.137	10.32543
Se	11.25889	11.13524	18.09691
Se	20.13184	11.13784	17.92041
Se	20.73086	18.08021	15.30163
Se	12.97129	18.07986	11.11525

Se	13.22482	18.07862	19.93107
Se	19.40074	15.51769	12.19412
Se	10.94561	15.51785	13.82017
Se	16.58179	15.51828	20.3331
Se	17.29788	11.32274	21.92407
Se	20.42609	11.32286	10.78055
Se	9.20998	11.3217	13.64087
Se	16.97231	18.97428	13.39373
Se	13.196	18.97445	15.32675
Se	16.75783	18.97456	17.63045
Se	17.7517	11.67104	14.14414
Se	13.45974	11.67106	14.27418
Se	15.71963	11.67177	17.92836
Se	22.81462	15.11282	18.32629
Se	14.55211	15.11219	7.80066
Se	9.56632	15.10869	20.21741
Se	7.49022	13.52035	16.34873
Se	20.50248	13.52198	22.05785
Se	18.94061	13.52262	7.93725
Se	22.07561	13.34074	14.55492
Se	11.65495	13.33923	10.32409
Se	13.20022	13.3379	21.4659
Se	17.25698	17.86868	8.95907
Se	9.21487	17.86686	17.29708
Se	20.45725	17.86816	20.09049
Se	13.47217	15.07843	17.19123
Se	18.23579	15.07946	16.45792
Se	15.21948	15.07936	12.69834

Table S11 Coordinates of atoms in optimized structure of **n34_Cd_4Se_6@$Cd_{30}Se_{28}$_1**.

Particle Type	Coordinates (Angstroms)		
	X	Y	Z
Cd	16.04618	20.56675	15.5958
Cd	19.13471	11.404	15.59565
Cd	9.65503	13.31184	15.59547
Cd	14.93016	12.7684	10.49758
Cd	12.9382	16.27142	10.49728
Cd	16.96761	16.24334	10.49741
Cd	11.38732	19.22387	11.09953
Cd	20.29902	16.11289	11.09902
Cd	13.151	9.94873	11.09948
Cd	18.66534	18.7242	13.03773
Cd	16.23104	10.05555	13.03668
Cd	9.94201	16.50132	13.03711
Cd	18.84904	14.27714	18.0982
Cd	12.28765	12.12161	18.0978
Cd	13.70121	18.88214	18.0985
Cd	15.16508	19.29021	11.16559
Cd	18.47067	12.80661	11.16609
Cd	11.20272	13.18518	11.1668
Cd	9.53483	13.97353	19.01269
Cd	16.68071	20.34089	19.01305
Cd	18.62269	10.96617	19.01233
Cd	10.48168	16.72956	17.04657
Cd	18.59424	18.14305	17.04679
Cd	15.76117	10.40794	17.04648
Cd	11.98718	19.03862	14.44999
Cd	19.84228	15.68427	14.44993
Cd	13.00944	10.55805	14.44995
Cd	16.53711	16.85532	19.99899
Cd	15.67673	12.83329	19.99843
Cd	12.62456	15.5909	19.99898
Cd	16.95447	13.71216	14.23194
Cd	12.74513	14.044	14.23164
Cd	15.13759	17.52438	14.23157
Cd	14.94624	15.09339	17.029
Se	9.52282	11.80704	17.76279
Se	14.81017	21.4342	17.76328
Se	20.50442	12.0406	17.763
Se	14.35039	20.10971	13.57961

Se	19.58734	13.10184	13.58016
Se	10.89958	12.06976	13.58053
Se	17.19445	16.17759	13.26922
Se	14.76029	12.60353	13.26927
Se	12.88256	16.49897	13.26927
Se	19.04897	14.71218	9.45602
Se	12.56334	11.73152	9.45633
Se	13.22469	18.83944	9.45623
Se	17.493	9.4209	15.25724
Se	8.75999	15.72551	15.25709
Se	18.58434	20.13596	15.25731
Se	21.14198	17.51575	12.97238
Se	13.94514	8.51656	12.97206
Se	9.75087	19.25036	12.9728
Se	11.38017	19.17714	16.95556
Se	20.26432	16.14063	16.95572
Se	13.19214	9.96324	16.95567
Se	14.09363	17.70201	20.46305
Se	17.63071	14.52738	20.46265
Se	13.11392	13.0514	20.46224
Se	15.78703	17.52544	16.82367
Se	16.63091	13.14822	16.82389
Se	12.41942	14.60655	16.82352
Se	17.64193	18.8774	10.58541
Se	16.87488	10.86786	10.58518
Se	10.32082	15.53631	10.58565
Se	18.45023	18.74236	19.7239
Se	16.35362	10.23296	19.7234
Se	10.03426	16.30511	19.72377
Se	14.94503	15.09441	9.31646

Table S12 Coordinates of atoms in optimized structure of **n34_(CdSe)$_6$@(CdSe)$_{28}$_1**.

Particle Type	Coordinates (Angstroms)		
	X	Y	Z
Cd	14.91802	9.89076	12.48801
Cd	15.08166	20.10636	17.50377
Cd	18.98435	16.80644	18.5782
Cd	11.01515	13.19056	11.41304
Cd	12.47104	17.99139	19.09934
Cd	17.52845	12.0053	10.89304
Cd	17.07881	16.60275	14.93076
Cd	12.92049	13.39405	15.06127
Cd	20.60325	15.49825	15.72776
Cd	9.39569	14.49829	14.26428
Cd	9.76466	16.64129	17.14475
Cd	20.2346	13.35455	12.84785
Cd	15.80031	17.3715	19.59276
Cd	14.19949	12.62547	10.39939
Cd	12.74471	20.62016	14.81797
Cd	17.25431	9.37626	15.17472
Cd	19.41593	12.11867	15.99854
Cd	10.58306	17.878	13.9941
Cd	10.59413	10.9608	14.19045
Cd	19.40508	19.03605	15.8009
Cd	16.83433	10.26013	18.56289
Cd	13.16437	19.73744	11.42946
Cd	13.62607	15.96996	11.34686
Cd	16.37311	14.02739	18.64571
Cd	16.17411	20.43132	13.81957
Cd	13.82503	9.56609	16.17212
Cd	16.0078	18.85972	10.26797
Cd	13.99091	11.13673	19.72464
Cd	18.01499	15.53861	11.13833
Cd	11.9845	14.45778	18.85382
Cd	11.03187	11.17436	17.77522
Cd	18.96697	18.82205	12.21654
Cd	13.64276	16.88166	15.57054
Cd	16.35647	13.11497	14.42189
Se	18.88699	20.73577	13.92864
Se	11.11231	9.26107	16.06268
Se	12.89416	11.67934	12.90126
Se	17.10521	18.31772	17.09058

Se	14.60686	8.81199	18.60436
Se	15.3922	21.18502	11.38742
Se	18.14728	11.33267	13.47432
Se	11.85185	18.6638	16.51816
Se	11.05158	20.20595	12.89178
Se	18.94727	9.79088	17.10099
Se	8.91982	12.41082	12.74498
Se	21.07959	17.58613	17.2463
Se	21.64857	13.19747	15.02087
Se	8.35052	16.79897	14.97186
Se	10.65425	13.57907	16.50471
Se	19.345	16.41769	13.48734
Se	14.37895	19.53732	19.97533
Se	15.62062	10.45954	10.01649
Se	17.91593	14.40961	16.44666
Se	12.08294	15.58711	13.54548
Se	19.60284	13.49488	10.34496
Se	10.39688	16.5016	19.64757
Se	12.36791	14.20732	9.51213
Se	17.6322	15.78983	20.47962
Se	11.62323	12.14419	20.09676
Se	18.37533	17.85222	9.89511
Se	15.18428	8.11424	14.32906
Se	14.8147	21.88282	15.66286
Se	16.35885	12.08921	20.39566
Se	13.63959	17.90813	9.5968
Se	14.21666	15.65443	17.9372
Se	15.78273	14.34222	12.05511
Se	14.83016	12.15554	16.36621
Se	15.16895	17.84126	13.62608

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