Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for:

Computational investigations on the structural and electronic properties of CdnTen (n = 1-17) quantum dots

*Muhammad Imran**[,a], Muhammad Jawwad Saif [a], Aleksey E. Kuznetsov[b], Nazeran Idrees[c], Javed Iqbal[d], Asif Ali Tahir[e]*

[a]Department of Applied Chemistry, Government College University Faisalabad – Pakistan

[b]Departamento de Química, Universidad Técnica Federico Santa María, Av. Santa María 6400, Vitacura, Santiago, Chile

[c]Department of Mathematics, Government College University Faisalabad – Pakistan

[d]Department of Chemistry, University of Agriculture, Faisalabad – Pakistan

[e]Environment and Sustainability Institute, University of Exeter, Penryn campus, TR 9FE, UK

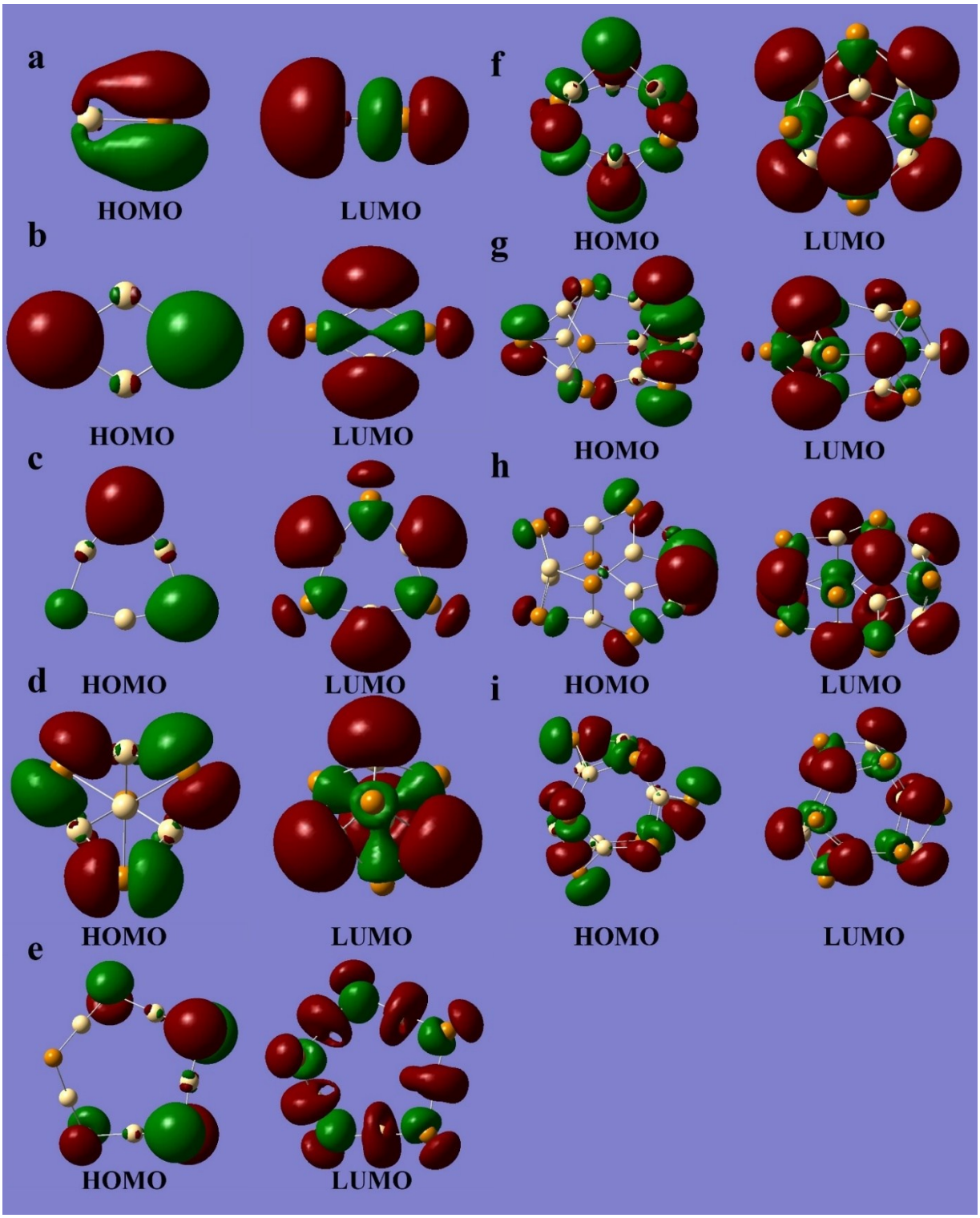

Figure S1. HOMO and LUMO of most stable lowest-energy clusters Cd_nTe_n (n=1-9).

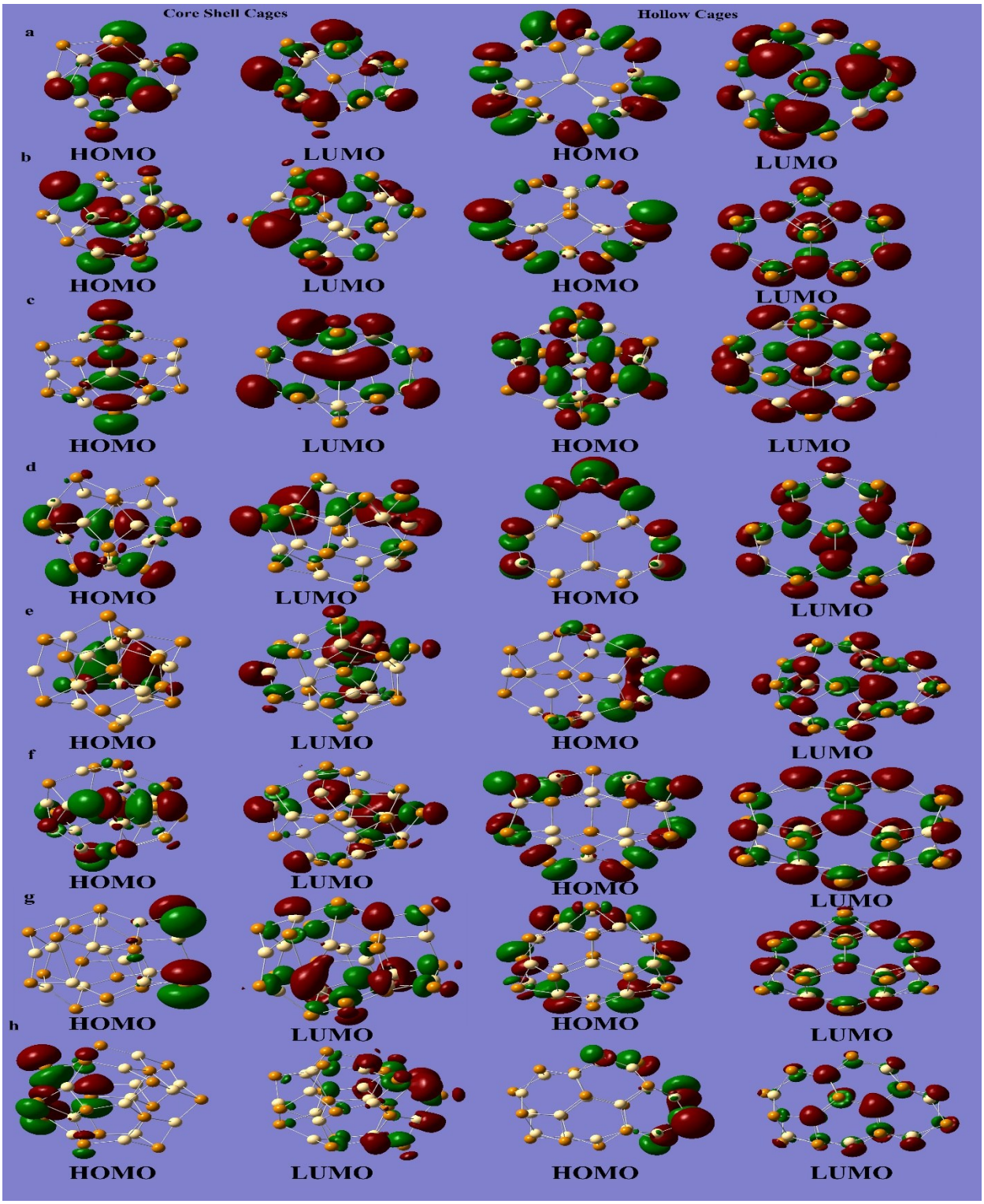

Figure S2. HOMO and LUMO of lowest-energy core-shell cage and hollow cage structures Cd_nTe_n (n=10-17).

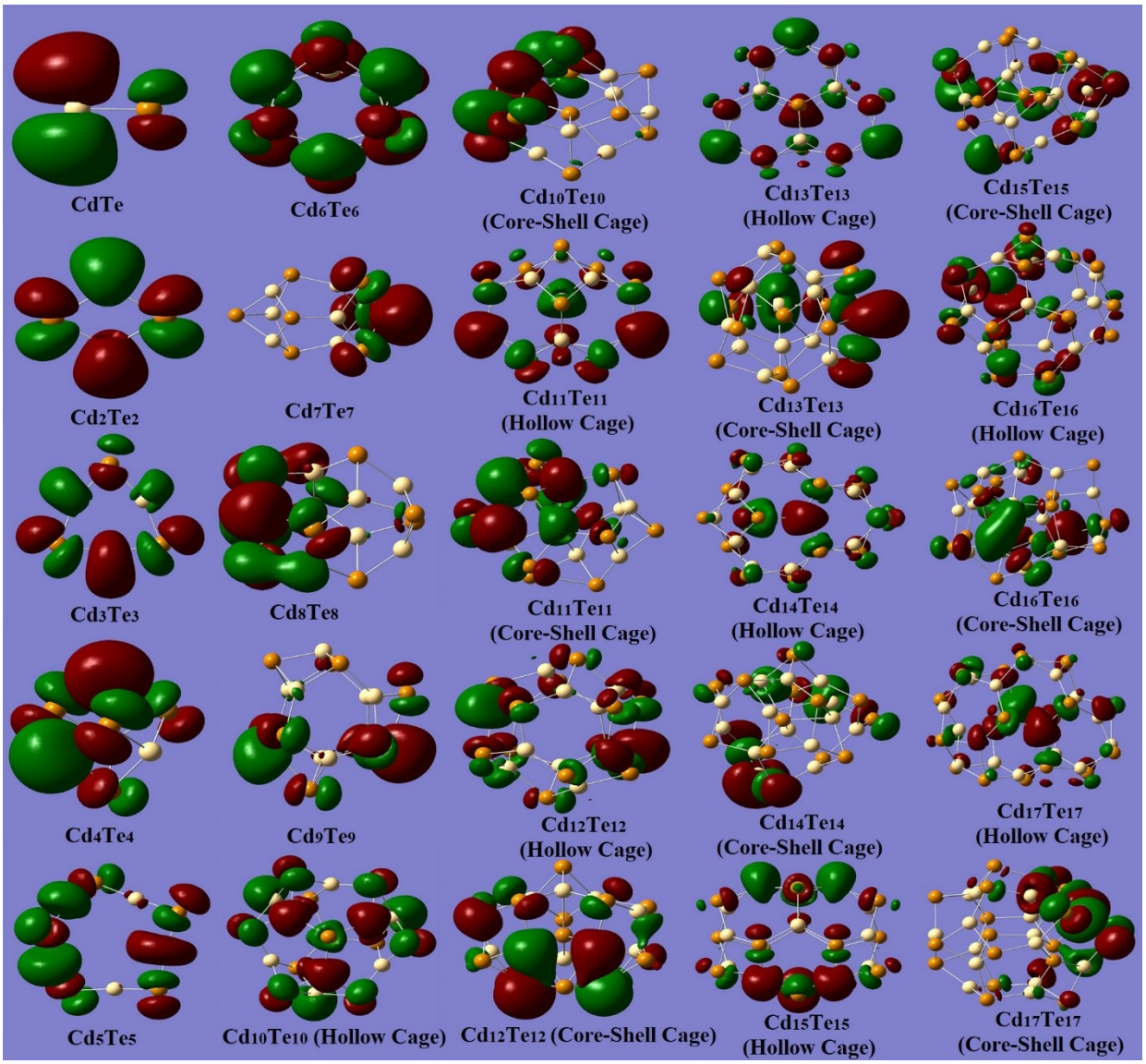

Figure S3. Plots of the LUMO+1 for clusters Cd_nTe_n (n=1-17).

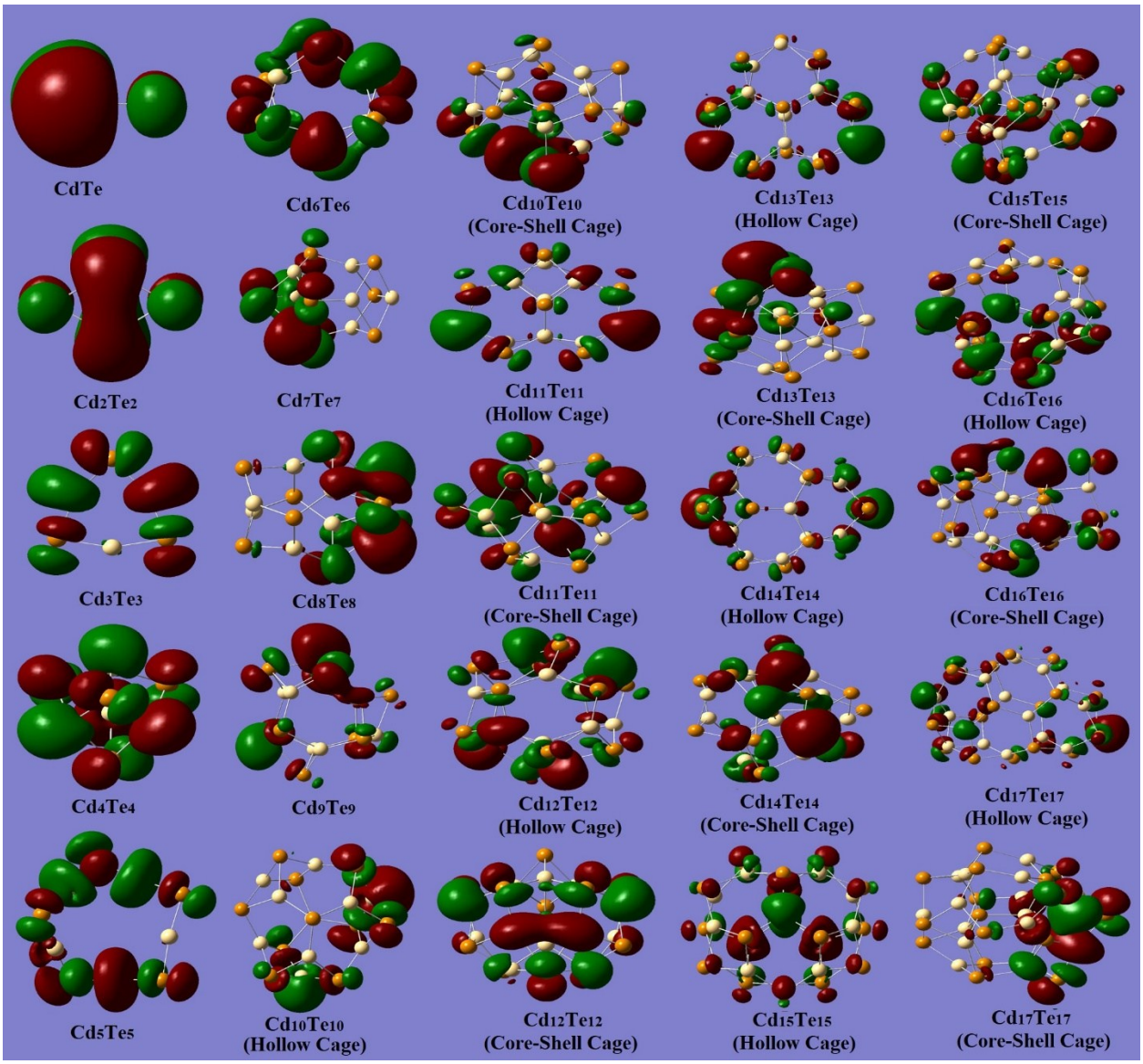

Figure S4. Plots of the LUMO+2 for clusters Cd_nTe_n (n=1-17).

Table S1. The binding energy (*Eb*) in eV per CdTe unit, point groups, HOMO values, LUMO values and HOMO-LUMO gaps calculated with B3LYP/Lanl2dz level of theory for the lowest energy optimized structures of Cd_nTe_n (n=1-17), the hollow cage and endohedral (core-shell) cage structures (n=10-17).

Clusters	Point Group	Binding Energy (*Eb*) (eV/unit)	HOMO (eV)	LUMO (eV)	HOMO-LUMO Gap (eV)
Cd_1Te_1	$C_{\infty v}$	1.66	-5.52	-4.27	1.25
Cd_2Te_2	D_{2h}	3.12	-5.61	-3.47	2.13
Cd_3Te_3	C_{3h}	3.74	-6.04	-2.94	3.11
Cd_4Te_4	T_d	3.81	-6.19	-3.22	2.97
Cd_5Te_5	C_1	3.86	-6.15	-2.86	3.29
Cd_6Te_6	S_6	4.07	-6.15	-3.1	3.05
Cd_7Te_7	C_{3v}	4.08	-6.19	-3.21	2.97
Cd_8Te_8	S_4	4.17	-6.2	-3.11	3.09
Cd_9Te_9	C_{3h}	4.21	-6.27	-3.13	3.14
$Cd_{10}Te_{10}$(Core-Shell Cage)	C_1	4.13	-5.95	-3.09	2.86
$Cd_{10}Te_{10}$ (Hollow Cage)	C_3	4.21	-6.2	-3.21	2.99
$Cd_{11}Te_{11}$(Core-Shell Cage)	C_1	4.19	-6.03	-3.13	2.9
$Cd_{11}Te_{11}$(Hollow Cage)	C_s	4.25	-6.26	-3.19	3.08
$Cd_{12}Te_{12}$(Core-Shell Cage)	C_1	4.2	-6.03	-3.23	2.8
$Cd_{12}Te_{12}$(Hollow Cage)	C_i	4.3	-6.5	-3.17	3.33
$Cd_{13}Te_{13}$(Core-Shell Cage)	C_1	4.29	-6.16	-4.04	2.12
$Cd_{13}Te_{13}$(Hollow Cage)	C_3	4.25	-6.24	-3.3	2.94
$Cd_{14}Te_{14}$(Core-Shell Cage)	C_1	4.25	-5.78	-3.2	2.58
$Cd_{14}Te_{14}$(Hollow Cage)	C_s	4.29	-6.31	-3.27	3.04
$Cd_{15}Te_{15}$(Core-Shell Cage)	C_1	4.25	-6.23	-3.37	2.86
$Cd_{15}Te_{15}$(Hollow Cage)	C_{3h}	4.32	-6.43	-3.27	3.16
$Cd_{16}Te_{16}$(Core-Shell Cage)	C_1	4.24	-5.71	-3.33	2.38
$Cd_{16}Te_{16}$(Hollow Cage)	C_1	4.32	-6.39	-3.32	3.08
$Cd_{17}Te_{17}$(Core-Shell Cage)	C_3	4.28	-5.98	-3.3	2.68
$Cd_{17}Te_{17}$(Hollow Cage)	C_1	4.31	-6.33	-3.34	2.99

Table S2. The binding energy (*Eb*) in eV per CdTe unit, point groups calculated with MP2/Def2-TZVP level of theory for the lowest energy optimized structures of Cd_nTe_n (n=1-17), the hollow cage and endohedral (core-shell) cage structures (n=10-17).

Clusters	Point Group	Binding Energy (*Eb*) (eV/unit)
Cd_1Te_1	$C_{\infty v}$	2.03
Cd_2Te_2	D_{2h}	3.76
Cd_3Te_3	C_{3h}	4.46
Cd_4Te_4	T_d	4.66
Cd_5Te_5	C_1	4.56
Cd_6Te_6	S_6	5
Cd_7Te_7	C_{3v}	5.02
Cd_8Te_8	S_4	5.13
Cd_9Te_9	C_{3h}	5.18
$Cd_{10}Te_{10}$(Core-Shell Cage)	C_1	5.18
$Cd_{10}Te_{10}$ (Hollow Cage)	C_3	4.96
$Cd_{11}Te_{11}$(Core-Shell Cage)	C_1	5.26
$Cd_{11}Te_{11}$(Hollow Cage)	C_s	5.23
$Cd_{12}Te_{12}$(Core-Shell Cage)	C_1	5.29
$Cd_{12}Te_{12}$(Hollow Cage)	C_i	5.26
$Cd_{13}Te_{13}$(Core-Shell Cage)	C_1	5.4
$Cd_{13}Te_{13}$(Hollow Cage)	C_3	5.24
$Cd_{14}Te_{14}$(Core-Shell Cage)	C_1	5.34
$Cd_{14}Te_{14}$(Hollow Cage)	C_s	5.26
$Cd_{15}Te_{15}$(Core-Shell Cage)	C_1	5.38
$Cd_{15}Te_{15}$(Hollow Cage)	C_{3h}	5.26
$Cd_{16}Te_{16}$(Core-Shell Cage)	C_1	5.37
$Cd_{16}Te_{16}$(Hollow Cage)	C_1	5.29
$Cd_{17}Te_{17}$(Core-Shell Cage)	C_3	5.38
$Cd_{17}Te_{17}$(Hollow Cage)	C_1	5.3