Electronic supplementary information for:

Chemical trends in the optical properties of rocksalt nanoparticles

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ESI-1 structural data

Table S1 *Distances between corner ions on the same face, given in Å, as calculated for structures optimised using BHLYP.*

BHLYP	MgO	CaO	SrO	MgS	MgSe	CdO
M-X corner to corner	5.87	6.76	7.24	7.29	7.68	6.52
X-X diagonal	8.42	9.523	10.13	10.69	11.32	9.28
M-M diagonal	8.17	9.59	10.34	9.89	10.35	9.16

Table S2 *Distances between corner ions on the same face, given in Å, as calculated for structures optimised using the B3LYP.*

B3LYP	MgO	CaO	SrO	MgS	MgSe	CdO
M-X corner to corner	5.93	6.79	7.29	7.33	7.73	6.60
X-X diagonal	8.52	9.57	10.20	10.77	11.40	9.41
M-M diagonal	8.26	9.64	10.41	9.94	10.41	9.26

From the data of table S1 and S2, it can be seen that the clusters are increasing in size as the ions become heavier. For the cases that the cation (M) are larger than the anion (X), the M-M distance across the face is larger than the X-X distance and vice versa.

ESI-2 Spectra

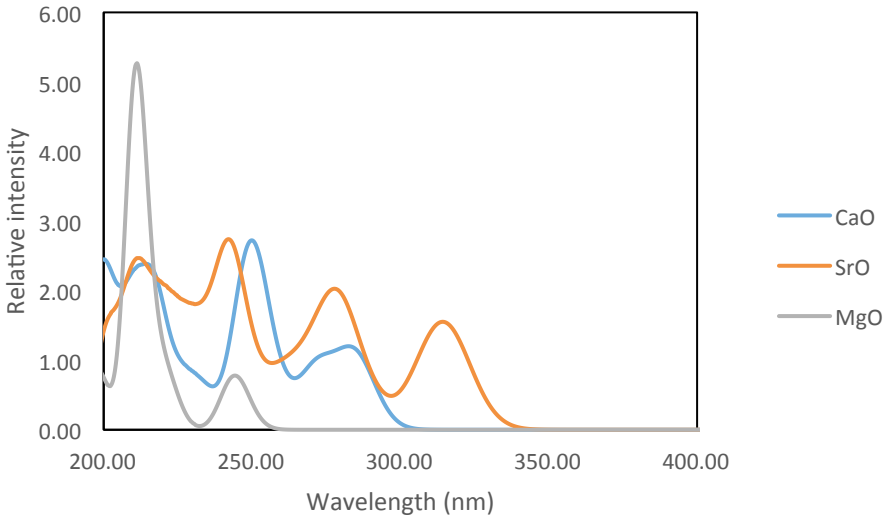

Fig. S1 *Unshifted TD-B3LYP spectra for the $(MgO)_{32}$, $(CaO)_{32}$ and $(SrO)_{32}$ nanoparticles.*

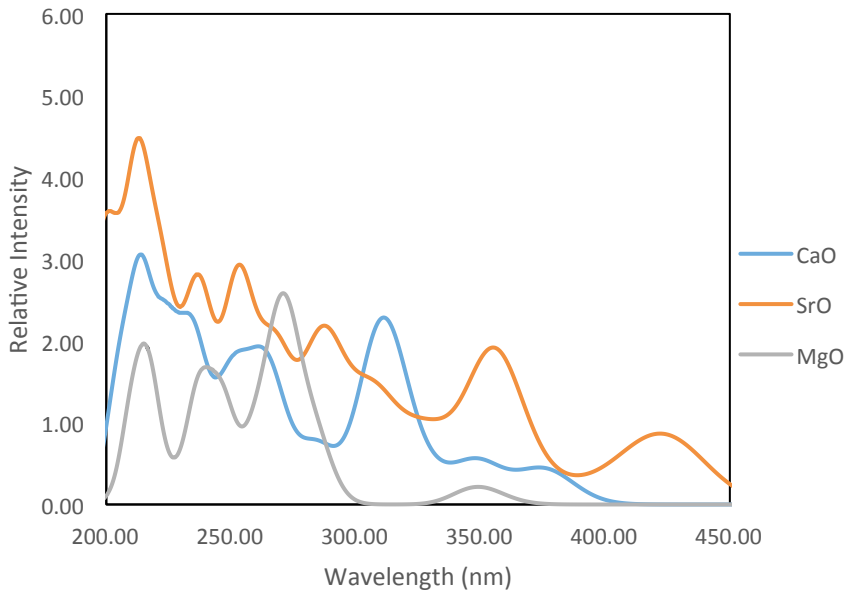

Fig. S2 *TD-B3LYP spectra for the $(MgO)_{32}$, $(CaO)_{32}$ and $(SrO)_{32}$ nanoparticles.*

ESI-3 Density Differences

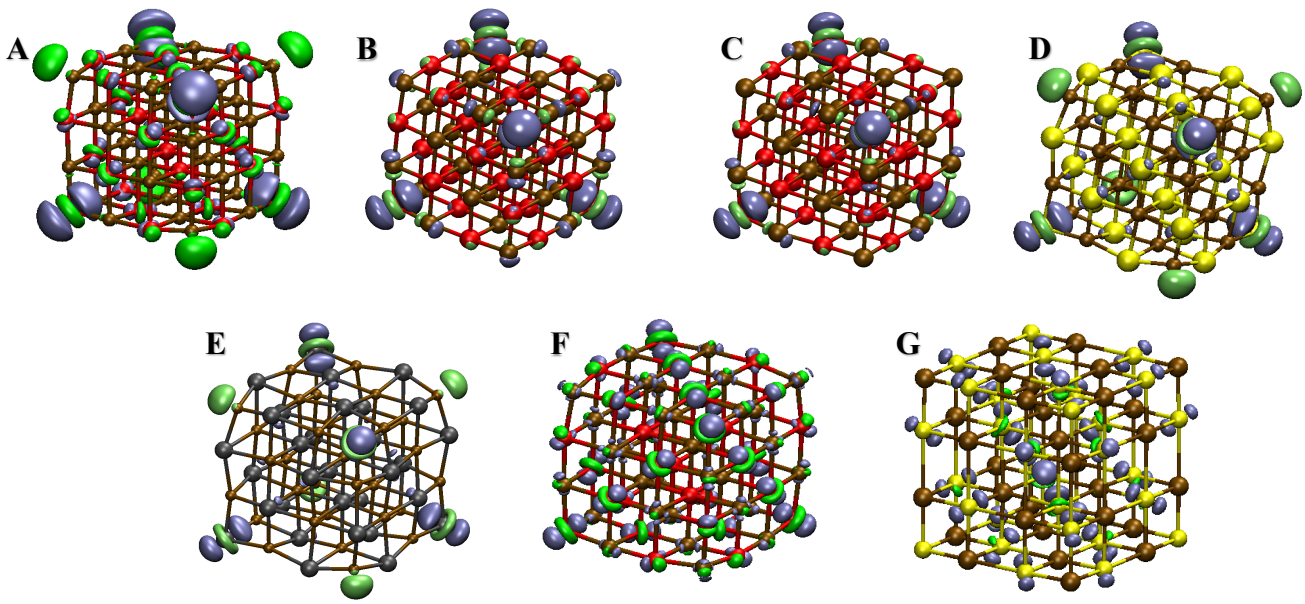

Fig. S3 *TD-B3LYP Electron density differences between the ground and lowest t_2 excited state for A MgO, B CaO, C SrO, D MgS, E MgSe, F CdO and G PbS. Red spheres are oxygen atoms, brown are magnesium (or calcium/strontium/cadmium/lead) atoms, yellow spheres are sulphur atoms, black spheres are selenium atoms. Green shows gain in electron density (excited electron), blue shows loss in electron density (hole). Same contour value (0.001) used in all figures.*

ESI-4 Ground and Excited State Charges

Table S3 *Ground (S0) and Excited (S1) state NBO charges for $(MgO)_{32}$ calculated using TD-BHLYP and TD-B3LYP*

	BHLYP		B3LYP	
atom	GS	ES	GS	ES
1 mg	1.82616	1.78011	1.80437	1.80004
2 o	-1.81042	-1.81107	-1.78555	-1.7884
3 o	-1.82342	-1.82132	-1.80755	-1.80514
4 mg	1.80892	1.8055	1.7918	1.78647
5 mg	1.80892	1.8055	1.7918	1.78647
6 o	-1.82342	-1.82132	-1.80755	-1.80514
7 o	-1.81042	-1.81107	-1.78555	-1.7884
8 mg	1.82616	1.78011	1.80437	1.80004
9 mg	1.8259	1.79208	1.79379	1.66047
10 o	-1.81042	-1.81107	-1.78555	-1.7884
11 mg	1.82616	1.78011	1.80437	1.80004
12 o	-1.79773	-1.61586	-1.76657	-1.59975
13 mg	1.8259	1.79208	1.79379	1.66047
14 o	-1.81042	-1.81107	-1.78555	-1.7884
15 mg	1.82616	1.78011	1.80437	1.80004
16 o	-1.79773	-1.61586	-1.76657	-1.59975
17 mg	1.82616	1.78011	1.80437	1.80004
18 o	-1.81042	-1.81107	-1.78555	-1.7884
19 o	-1.82342	-1.82132	-1.80755	-1.80514
20 mg	1.80892	1.8055	1.7918	1.78647
21 mg	1.80892	1.8055	1.7918	1.78647
22 o	-1.82342	-1.82132	-1.80755	-1.80514
23 o	-1.81042	-1.81107	-1.78555	-1.7884
24 mg	1.82616	1.78011	1.80437	1.80004
25 mg	1.8259	1.79208	1.79379	1.66047
26 o	-1.81042	-1.81107	-1.78555	-1.7884
27 mg	1.82616	1.78011	1.80437	1.80004
28 o	-1.79773	-1.61586	-1.76657	-1.59975
29 mg	1.8259	1.79208	1.79379	1.66047

30 o	-1.81042	-1.81107	-1.78555	-1.7884
31 mg	1.82616	1.78011	1.80437	1.80004
32 o	-1.79773	-1.61586	-1.76657	-1.59975
33 o	-1.81042	-1.81107	-1.78555	-1.7884
34 mg	1.80892	1.8055	1.7918	1.78647
35 o	-1.82342	-1.82132	-1.80755	-1.80514
36 mg	1.82616	1.78011	1.80437	1.80004
37 mg	1.82616	1.78011	1.80437	1.80004
38 o	-1.82342	-1.82132	-1.80755	-1.80514
39 mg	1.80892	1.8055	1.7918	1.78647
40 o	-1.81042	-1.81107	-1.78555	-1.7884
41 o	-1.81042	-1.81107	-1.78555	-1.7884
42 mg	1.80892	1.8055	1.7918	1.78647
43 o	-1.82342	-1.82132	-1.80755	-1.80514
44 mg	1.82616	1.78011	1.80437	1.80004
45 mg	1.82616	1.78011	1.80437	1.80004
46 o	-1.82342	-1.82132	-1.80755	-1.80514
47 mg	1.80892	1.8055	1.7918	1.78647
48 o	-1.81042	-1.81107	-1.78555	-1.7884
49 mg	1.80892	1.8055	1.7918	1.78647
50 o	-1.82342	-1.82132	-1.80755	-1.80514
51 o	-1.82342	-1.82132	-1.80755	-1.80514
52 mg	1.80892	1.8055	1.7918	1.78647
53 o	-1.82934	-1.84238	-1.82048	-1.83765
54 mg	1.79747	1.80649	1.78406	1.79799
55 mg	1.79747	1.80649	1.78406	1.79799
56 o	-1.82934	-1.84238	-1.82048	-1.83765
57 mg	1.79747	1.80649	1.78406	1.79799
58 o	-1.82934	-1.84238	-1.82048	-1.83765
59 o	-1.82934	-1.84238	-1.82048	-1.83765
60 mg	1.79747	1.80649	1.78406	1.79799
61 o	-1.82342	-1.82132	-1.80755	-1.80514
62 mg	1.80892	1.8055	1.7918	1.78647
63 mg	1.80892	1.8055	1.7918	1.78647
64 o	-1.82342	-1.82132	-1.80755	-1.80514

Table S4 *Ground (S0) and Excited (S1) state NBO charges for $(CaO)_{32}$ calculated using TD-BHLYP and TD-B3LYP.*

	BHLYP		B3LYP	
atom	GS	ES	GS	ES
1 ca	1.81864	1.76752	1.77807	1.77822
2 o	-1.80807	-1.80476	-1.76822	-1.7671
3 o	-1.80148	-1.80916	-1.76466	-1.77815
4 ca	1.79695	1.79662	1.76225	1.76206
5 ca	1.79695	1.79662	1.76225	1.76206
6 o	-1.80148	-1.80916	-1.76466	-1.77815
7 o	-1.80807	-1.80476	-1.76822	-1.7671
8 ca	1.81864	1.76752	1.77807	1.77822
9 ca	1.79989	1.78526	1.74713	1.62779
10 o	-1.80807	-1.80476	-1.76822	-1.7671
11 ca	1.81864	1.76752	1.77807	1.77822
12 o	-1.80529	-1.6236	-1.76084	-1.59922
13 ca	1.79989	1.78526	1.74713	1.62779
14 o	-1.80807	-1.80476	-1.76822	-1.7671
15 ca	1.81864	1.76752	1.77807	1.77822
16 o	-1.80529	-1.6236	-1.76084	-1.59922
17 ca	1.81864	1.76752	1.77807	1.77822
18 o	-1.80807	-1.80476	-1.76822	-1.7671
19 o	-1.80148	-1.80916	-1.76466	-1.77815
20 ca	1.79695	1.79662	1.76225	1.76206
21 ca	1.79695	1.79662	1.76225	1.76206
22 o	-1.80148	-1.80916	-1.76466	-1.77815
23 o	-1.80807	-1.80476	-1.76822	-1.7671
24 ca	1.81864	1.76752	1.77807	1.77822
25 ca	1.79989	1.78526	1.74713	1.62779
26 o	-1.80807	-1.80476	-1.76822	-1.7671
27 ca	1.81864	1.76752	1.77807	1.77822
28 o	-1.80529	-1.6236	-1.76084	-1.59922
29 ca	1.79989	1.78526	1.74713	1.62779
30 o	-1.80807	-1.80476	-1.76822	-1.7671
31 ca	1.81864	1.76752	1.77807	1.77822

32 o	-1.80529	-1.6236	-1.76084	-1.59922
33 o	-1.80807	-1.80476	-1.76822	-1.7671
34 ca	1.79695	1.79662	1.76225	1.76206
35 o	-1.80148	-1.80916	-1.76466	-1.77815
36 ca	1.81864	1.76752	1.77807	1.77822
37 ca	1.81864	1.76752	1.77807	1.77822
38 o	-1.80148	-1.80916	-1.76466	-1.77815
39 ca	1.79695	1.79662	1.76225	1.76206
40 o	-1.80807	-1.80476	-1.76822	-1.7671
41 o	-1.80807	-1.80476	-1.76822	-1.7671
42 ca	1.79695	1.79662	1.76225	1.76206
43 o	-1.80148	-1.80916	-1.76466	-1.77815
44 ca	1.81864	1.76752	1.77807	1.77822
45 ca	1.81864	1.76752	1.77807	1.77822
46 o	-1.80148	-1.80916	-1.76466	-1.77815
47 ca	1.79695	1.79662	1.76225	1.76206
48 o	-1.80807	-1.80476	-1.76822	-1.7671
49 ca	1.79695	1.79662	1.76225	1.76206
50 o	-1.80148	-1.80916	-1.76466	-1.77815
51 o	-1.80148	-1.80916	-1.76466	-1.77815
52 ca	1.79695	1.79662	1.76225	1.76206
53 o	-1.78023	-1.79961	-1.74363	-1.78362
54 ca	1.76749	1.78728	1.73503	1.76995
55 ca	1.7675	1.78727	1.73503	1.76995
56 o	-1.78023	-1.79961	-1.74363	-1.78362
57 ca	1.7675	1.78727	1.73503	1.76995
58 o	-1.78023	-1.79961	-1.74363	-1.78362
59 o	-1.78023	-1.79961	-1.74363	-1.78362
60 ca	1.7675	1.78727	1.73503	1.76995
61 o	-1.80148	-1.80916	-1.76466	-1.77815
62 ca	1.79695	1.79662	1.76225	1.76206
63 ca	1.79695	1.79662	1.76225	1.76206
64 o	-1.80148	-1.80916	-1.76466	-1.77815

Table S5 *Ground (S0) and Excited (S1) state NBO charges for $(SrO)_{32}$ calculated using TD-BHLYP and TD-B3LYP.*

	BHLYP		B3LYP	
atom	GS	ES	GS	ES
1 sr	1.83968	1.79128	-1.79038	1.80193
2 o	-1.8274	-1.82448	-1.79038	-1.78954
3 o	-1.82918	-1.84118	-1.79038	-1.80741
4 sr	1.82466	1.82866	-1.79038	1.79412
5 sr	1.82466	1.82866	-1.79038	1.79412
6 o	-1.82918	-1.84118	-1.79038	-1.80741
7 o	-1.8274	-1.82448	-1.79038	-1.78954
8 sr	1.83968	1.79128	-1.79038	1.80193
9 sr	1.8129	1.80534	-1.79038	1.6763
10 o	-1.8274	-1.82448	-1.79038	-1.78954
11 sr	1.83968	1.79128	-1.79038	1.80193
12 o	-1.82782	-1.64841	-1.79038	-1.63026
13 sr	1.8129	1.80534	-1.79038	1.6763
14 o	-1.8274	-1.82448	-1.79038	-1.78954
15 sr	1.83968	1.79128	-1.79038	1.80193
16 o	-1.82782	-1.64841	-1.79038	-1.63026
17 sr	1.83968	1.79128	-1.79038	1.80193
18 o	-1.8274	-1.82448	-1.79038	-1.78954
19 o	-1.82918	-1.84118	-1.79038	-1.80741
20 sr	1.82466	1.82866	-1.79038	1.79412
21 sr	1.82466	1.82866	-1.79038	1.79412
22 o	-1.82918	-1.84118	-1.79038	-1.80741
23 o	-1.8274	-1.82448	-1.79038	-1.78954
24 sr	1.83968	1.79128	-1.79038	1.80193
25 sr	1.8129	1.80534	-1.79038	1.6763
26 o	-1.8274	-1.82448	-1.79038	-1.78954
27 sr	1.83968	1.79128	-1.79038	1.80193
28 o	-1.82782	-1.64841	-1.79038	-1.63026
29 sr	1.8129	1.80534	-1.79038	1.6763
30 o	-1.8274	-1.82448	-1.79038	-1.78954
31 sr	1.83968	1.79128	-1.79038	1.80193

32 o	-1.82782	-1.64841	-1.79038	-1.63026
33 o	-1.8274	-1.82448	-1.79038	-1.78954
34 sr	1.82466	1.82866	-1.79038	1.79412
35 o	-1.82918	-1.84118	-1.79038	-1.80741
36 sr	1.83968	1.79128	-1.79038	1.80193
37 sr	1.83968	1.79128	-1.79038	1.80193
38 o	-1.82918	-1.84118	-1.79038	-1.80741
39 sr	1.82466	1.82866	-1.79038	1.79412
40 o	-1.8274	-1.82448	-1.79038	-1.78954
41 o	-1.8274	-1.82448	-1.79038	-1.78954
42 sr	1.82466	1.82866	-1.79038	1.79412
43 o	-1.82918	-1.84118	-1.79038	-1.80741
44 sr	1.83968	1.79128	-1.79038	1.80193
45 sr	1.83968	1.79128	-1.79038	1.80193
46 o	-1.82918	-1.84118	-1.79038	-1.80741
47 sr	1.82466	1.82866	-1.79038	1.79412
48 o	-1.8274	-1.82448	-1.79038	-1.78954
49 sr	1.82466	1.82866	-1.79038	1.79412
50 o	-1.82918	-1.84118	-1.79038	-1.80741
51 o	-1.82918	-1.84118	-1.79038	-1.80741
52 sr	1.82466	1.82866	-1.79038	1.79412
53 o	-1.8143	-1.84116	-1.79038	-1.8268
54 sr	1.80594	1.82139	-1.79038	1.78347
55 sr	1.80593	1.82139	-1.79038	1.78346
56 o	-1.8143	-1.84116	-1.79038	-1.8268
57 sr	1.80593	1.82139	-1.79038	1.78346
58 o	-1.8143	-1.84116	-1.79038	-1.8268
59 o	-1.8143	-1.84116	-1.79038	-1.8268
60 sr	1.80593	1.82139	-1.79038	1.78346
61 o	-1.82918	-1.84118	-1.79038	-1.80741
62 sr	1.82466	1.82866	-1.79038	1.79412
63 sr	1.82466	1.82866	-1.79038	1.79412
64 o	-1.82918	-1.84118	-1.79038	-1.80741

Table S6 *Ground (S0) and Excited (S1) state NBO charges for $(MgS)_{32}$ calculated using TD-BHLYP and TD-B3LYP.*

	BHLYP		B3LYP	
atom	GS	ES	GS	ES
1 mg	1.69637	1.65427	1.66872	1.65361
2 s	-1.66803	-1.66676	-1.63726	-1.63795
3 s	-1.72286	-1.70644	-1.70158	-1.68071
4 mg	1.69445	1.69217	1.66969	1.66388
5 mg	1.69445	1.69217	1.66969	1.66388
6 s	-1.72286	-1.70644	-1.70158	-1.68071
7 s	-1.66803	-1.66676	-1.63726	-1.63795
8 mg	1.69637	1.65427	1.66872	1.65361
9 mg	1.69806	1.64787	1.66668	1.54781
10 s	-1.66803	-1.66676	-1.63726	-1.63795
11 mg	1.69637	1.65427	1.66872	1.65361
12 s	-1.603	-1.46496	-1.56077	-1.44228
13 mg	1.69806	1.64787	1.66668	1.54781
14 s	-1.66803	-1.66676	-1.63726	-1.63795
15 mg	1.69637	1.65427	1.66872	1.65361
16 s	-1.603	-1.46496	-1.56077	-1.44228
17 mg	1.69637	1.65427	1.66872	1.65361
18 s	-1.66803	-1.66676	-1.63726	-1.63795
19 s	-1.72286	-1.70644	-1.70158	-1.68071
20 mg	1.69445	1.69217	1.66969	1.66388
21 mg	1.69445	1.69217	1.66969	1.66388
22 s	-1.72286	-1.70644	-1.70158	-1.68071
23 s	-1.66803	-1.66676	-1.63726	-1.63795
24 mg	1.69637	1.65427	1.66872	1.65361
25 mg	1.69806	1.64787	1.66668	1.54781
26 s	-1.66803	-1.66676	-1.63726	-1.63795
27 mg	1.69637	1.65427	1.66872	1.65361
28 s	-1.603	-1.46496	-1.56077	-1.44228
29 mg	1.69806	1.64787	1.66668	1.54781
30 s	-1.66803	-1.66676	-1.63726	-1.63795
31 mg	1.69637	1.65427	1.66872	1.65361

32 s	-1.603	-1.46496	-1.56077	-1.44228
33 s	-1.66803	-1.66676	-1.63726	-1.63795
34 mg	1.69445	1.69217	1.66969	1.66388
35 s	-1.72286	-1.70644	-1.70158	-1.68071
36 mg	1.69637	1.65427	1.66872	1.65361
37 mg	1.69637	1.65427	1.66872	1.65361
38 s	-1.72286	-1.70644	-1.70158	-1.68071
39 mg	1.69445	1.69217	1.66969	1.66388
40 s	-1.66803	-1.66676	-1.63726	-1.63795
41 s	-1.66803	-1.66676	-1.63726	-1.63795
42 mg	1.69445	1.69217	1.66969	1.66388
43 s	-1.72286	-1.70644	-1.70158	-1.68071
44 mg	1.69637	1.65427	1.66872	1.65361
45 mg	1.69637	1.65427	1.66872	1.65361
46 s	-1.72286	-1.70644	-1.70158	-1.68071
47 mg	1.69445	1.69217	1.66969	1.66388
48 s	-1.66803	-1.66676	-1.63726	-1.63795
49 mg	1.69445	1.69217	1.66969	1.66388
50 s	-1.72286	-1.70644	-1.70158	-1.68071
51 s	-1.72286	-1.70644	-1.70158	-1.68071
52 mg	1.69445	1.69217	1.66969	1.66388
53 s	-1.76864	-1.76828	-1.75919	-1.75798
54 mg	1.67377	1.66565	1.65459	1.65596
55 mg	1.67377	1.66565	1.65459	1.65596
56 s	-1.76864	-1.76828	-1.75919	-1.75798
57 mg	1.67377	1.66565	1.65459	1.65596
58 s	-1.76864	-1.76828	-1.75919	-1.75798
59 s	-1.76864	-1.76828	-1.75919	-1.75798
60 mg	1.67377	1.66565	1.65459	1.65596
61 s	-1.72286	-1.70644	-1.70158	-1.68071
62 mg	1.69445	1.69217	1.66969	1.66388
63 mg	1.69445	1.69217	1.66969	1.66388
64 s	-1.72286	-1.70644	-1.70158	-1.68071

Table S7 *Ground (S0) and Excited (S1) state NBO charges for* $(MgSe)_{32}$ *calculated using TD-BHLYP and TD-B3LYP.*

	BHLYP		B3LYP	
atom	GS	ES	GS	ES
1 mg	1.65627	1.62031	1.62327	1.60363
2 se	-1.62765	-1.6238	-1.5914	-1.59015
3 se	-1.68852	-1.66568	-1.66239	-1.63697
4 mg	1.65658	1.65357	1.62657	1.62097
5 mg	1.65658	1.65357	1.62657	1.62097
6 se	-1.68852	-1.66568	-1.66239	-1.63697
7 se	-1.62765	-1.6238	-1.5914	-1.59015
8 mg	1.65627	1.62031	1.62327	1.60363
9 mg	1.66225	1.59242	1.62685	1.52086
10 se	-1.62765	-1.6238	-1.5914	-1.59015
11 mg	1.65627	1.62031	1.62327	1.60363
12 se	-1.54446	-1.43592	-1.49473	-1.40001
13 mg	1.66225	1.59242	1.62685	1.52086
14 se	-1.62765	-1.6238	-1.5914	-1.59015
15 mg	1.65627	1.62031	1.62327	1.60363
16 se	-1.54446	-1.43592	-1.49473	-1.40001
17 mg	1.65627	1.62031	1.62327	1.60363
18 se	-1.62765	-1.6238	-1.5914	-1.59015
19 se	-1.68852	-1.66568	-1.66239	-1.63697
20 mg	1.65658	1.65357	1.62657	1.62097
21 mg	1.65658	1.65357	1.62657	1.62097
22 se	-1.68852	-1.66568	-1.66239	-1.63697
23 se	-1.62765	-1.6238	-1.5914	-1.59015
24 mg	1.65627	1.62031	1.62327	1.60363
25 mg	1.66225	1.59242	1.62685	1.52086
26 se	-1.62765	-1.6238	-1.5914	-1.59015
27 mg	1.65627	1.62031	1.62327	1.60363
28 se	-1.54446	-1.43592	-1.49473	-1.40001
29 mg	1.66225	1.59242	1.62685	1.52086
30 se	-1.62765	-1.6238	-1.5914	-1.59015
31 mg	1.65627	1.62031	1.62327	1.60363

32 se	-1.54446	-1.43592	-1.49473	-1.40001
33 se	-1.62765	-1.6238	-1.5914	-1.59015
34 mg	1.65658	1.65357	1.62657	1.62097
35 se	-1.68852	-1.66568	-1.66239	-1.63697
36 mg	1.65627	1.62031	1.62327	1.60363
37 mg	1.65627	1.62031	1.62327	1.60363
38 se	-1.68852	-1.66568	-1.66239	-1.63697
39 mg	1.65658	1.65357	1.62657	1.62097
40 se	-1.62765	-1.6238	-1.5914	-1.59015
41 se	-1.62765	-1.6238	-1.5914	-1.59015
42 mg	1.65658	1.65357	1.62657	1.62097
43 se	-1.68852	-1.66568	-1.66239	-1.63697
44 mg	1.65627	1.62031	1.62327	1.60363
45 mg	1.65627	1.62031	1.62327	1.60363
46 se	-1.68852	-1.66568	-1.66239	-1.63697
47 mg	1.65658	1.65357	1.62657	1.62097
48 se	-1.62765	-1.6238	-1.5914	-1.59015
49 mg	1.65658	1.65357	1.62657	1.62097
50 se	-1.68852	-1.66568	-1.66239	-1.63697
51 se	-1.68852	-1.66568	-1.66239	-1.63697
52 mg	1.65658	1.65357	1.62657	1.62097
53 se	-1.74564	-1.74217	-1.73577	-1.72929
54 mg	1.63781	1.63248	1.61552	1.616
55 mg	1.63781	1.63248	1.61552	1.616
56 se	-1.74564	-1.74217	-1.73577	-1.72929
57 mg	1.63781	1.63248	1.61552	1.616
58 se	-1.74564	-1.74217	-1.73577	-1.72929
59 se	-1.74564	-1.74217	-1.73577	-1.72929
60 mg	1.63781	1.63248	1.61552	1.616
61 se	-1.68852	-1.66568	-1.66239	-1.63697
62 mg	1.65658	1.65357	1.62657	1.62097
63 mg	1.65658	1.65357	1.62657	1.62097
64 se	-1.68852	-1.66568	-1.66239	-1.63697

Table S8 *Ground (S0) and Excited (S1) state NBO charges for $(CdO)_{32}$ calculated using TD-BHLYP and TD-B3LYP.*

	BHLYP		B3LYP	
atom	GS	ES	GS	ES
1 cd	1.72014	1.70521	1.63845	1.62764
2 o	-1.68809	-1.6698	-1.59764	-1.58806
3 o	-1.76685	-1.74595	-1.69359	-1.67269
4 cd	1.73112	1.72142	1.65061	1.64348
5 cd	1.73112	1.72142	1.65061	1.64348
6 o	-1.76685	-1.74595	-1.69359	-1.67269
7 o	-1.68809	-1.6698	-1.59764	-1.58806
8 cd	1.72014	1.70521	1.63845	1.62764
9 cd	1.70037	1.62589	1.5998	1.53624
10 o	-1.68809	-1.6698	-1.59764	-1.58806
11 cd	1.72014	1.70521	1.63845	1.62764
12 o	-1.58991	-1.55426	-1.47304	-1.44262
13 cd	1.70037	1.62589	1.5998	1.53624
14 o	-1.68809	-1.6698	-1.59764	-1.58806
15 cd	1.72014	1.70521	1.63845	1.62764
16 o	-1.58991	-1.55426	-1.47304	-1.44262
17 cd	1.72014	1.70521	1.63845	1.62764
18 o	-1.68809	-1.6698	-1.59764	-1.58806
19 o	-1.76685	-1.74595	-1.69359	-1.67269
20 cd	1.73112	1.72142	1.65061	1.64348
21 cd	1.73112	1.72142	1.65061	1.64348
22 o	-1.76685	-1.74595	-1.69359	-1.67269
23 o	-1.68809	-1.6698	-1.59764	-1.58806
24 cd	1.72014	1.70521	1.63845	1.62764
25 cd	1.70037	1.62589	1.5998	1.53624
26 o	-1.68809	-1.6698	-1.59764	-1.58806
27 cd	1.72014	1.70521	1.63845	1.62764
28 o	-1.58991	-1.55426	-1.47304	-1.44262
29 cd	1.70037	1.62589	1.5998	1.53624
30 o	-1.68809	-1.6698	-1.59764	-1.58806
31 cd	1.72014	1.70521	1.63845	1.62764

32 o	-1.58991	-1.55426	-1.47304	-1.44262
33 o	-1.68809	-1.6698	-1.59764	-1.58806
34 cd	1.73112	1.72142	1.65061	1.64348
35 o	-1.76685	-1.74595	-1.69359	-1.67269
36 cd	1.72014	1.70521	1.63845	1.62764
37 cd	1.72014	1.70521	1.63845	1.62764
38 o	-1.76685	-1.74595	-1.69359	-1.67269
39 cd	1.73112	1.72142	1.65061	1.64348
40 o	-1.68809	-1.6698	-1.59764	-1.58806
41 o	-1.68809	-1.6698	-1.59764	-1.58806
42 cd	1.73112	1.72142	1.65061	1.64348
43 o	-1.76685	-1.74595	-1.69359	-1.67269
44 cd	1.72014	1.70521	1.63845	1.62764
45 cd	1.72014	1.70521	1.63845	1.62764
46 o	-1.76685	-1.74595	-1.69359	-1.67269
47 cd	1.73112	1.72142	1.65061	1.64348
48 o	-1.68809	-1.6698	-1.59764	-1.58806
49 cd	1.73112	1.72142	1.65061	1.64348
50 o	-1.76685	-1.74595	-1.69359	-1.67269
51 o	-1.76685	-1.74595	-1.69359	-1.67269
52 cd	1.73112	1.72142	1.65061	1.64348
53 o	-1.81527	-1.81725	-1.75764	-1.75964
54 cd	1.71584	1.71295	1.63742	1.63487
55 cd	1.71584	1.71295	1.63742	1.63487
56 o	-1.81527	-1.81725	-1.75764	-1.75964
57 cd	1.71584	1.71295	1.63742	1.63487
58 o	-1.81527	-1.81725	-1.75764	-1.75964
59 o	-1.81527	-1.81725	-1.75764	-1.75964
60 cd	1.71584	1.71295	1.63742	1.63487
61 o	-1.76685	-1.74595	-1.69359	-1.67269
62 cd	1.73112	1.72142	1.65061	1.64348
63 cd	1.73112	1.72142	1.65061	1.64348
64 o	-1.76685	-1.74595	-1.69359	-1.67269

Table S9 *Ground (S0) and Excited (S1) state NBO charges for $(PbS)_{32}$ calculated using TD-BHLYP and TD-B3LYP.*

	BHLYP		B3LYP	
atom	GS	ES	GS	ES
1 pb	1.16494	1.15192	1.12306	1.11333
2 s	-1.22072	-1.20021	-1.16745	-1.15054
3 s	-1.2235	-1.2048	-1.17672	-1.15631
4 pb	1.31834	1.29067	1.26651	1.23879
5 pb	1.31834	1.29067	1.26651	1.23879
6 s	-1.2235	-1.2048	-1.17672	-1.15631
7 s	-1.22072	-1.20021	-1.16745	-1.15054
8 pb	1.16494	1.15192	1.12306	1.11333
9 pb	1.0613	1.05692	1.01591	1.01978
10 s	-1.22072	-1.20021	-1.16745	-1.15054
11 pb	1.16494	1.15192	1.12306	1.11333
12 s	-1.08362	-1.07027	-1.03779	-1.01715
13 pb	1.0613	1.05692	1.01591	1.01978
14 s	-1.22072	-1.20021	-1.16745	-1.15054
15 pb	1.16494	1.15192	1.12306	1.11333
16 s	-1.08362	-1.07027	-1.03779	-1.01715
17 pb	1.16494	1.15192	1.12306	1.11333
18 s	-1.22072	-1.20021	-1.16745	-1.15054
19 s	-1.2235	-1.2048	-1.17672	-1.15631
20 pb	1.31834	1.29067	1.26651	1.23879
21 pb	1.31834	1.29067	1.26651	1.23879
22 s	-1.2235	-1.2048	-1.17672	-1.15631
23 s	-1.22072	-1.20021	-1.16745	-1.15054
24 pb	1.16494	1.15192	1.12306	1.11333
25 pb	1.0613	1.05692	1.01591	1.01978
26 s	-1.22072	-1.20021	-1.16745	-1.15054
27 pb	1.16494	1.15192	1.12306	1.11333
28 s	-1.08362	-1.07027	-1.03779	-1.01715
29 pb	1.0613	1.05692	1.01591	1.01978
30 s	-1.22072	-1.20021	-1.16745	-1.15054
31 pb	1.16494	1.15192	1.12306	1.11333

32 s	-1.08362	-1.07027	-1.03779	-1.01715
33 s	-1.22072	-1.20021	-1.16745	-1.15054
34 pb	1.31834	1.29067	1.26651	1.23879
35 s	-1.2235	-1.2048	-1.17672	-1.15631
36 pb	1.16494	1.15192	1.12306	1.11333
37 pb	1.16494	1.15192	1.12306	1.11333
38 s	-1.2235	-1.2048	-1.17672	-1.15631
39 pb	1.31834	1.29067	1.26651	1.23879
40 s	-1.22072	-1.20021	-1.16745	-1.15054
41 s	-1.22072	-1.20021	-1.16745	-1.15054
42 pb	1.31834	1.29067	1.26651	1.23879
43 s	-1.2235	-1.2048	-1.17672	-1.15631
44 pb	1.16494	1.15192	1.12306	1.11333
45 pb	1.16494	1.15192	1.12306	1.11333
46 s	-1.2235	-1.2048	-1.17672	-1.15631
47 pb	1.31834	1.29067	1.26651	1.23879
48 s	-1.22072	-1.20021	-1.16745	-1.15054
49 pb	1.31834	1.29067	1.26651	1.23879
50 s	-1.2235	-1.2048	-1.17672	-1.15631
51 s	-1.2235	-1.2048	-1.17672	-1.15631
52 pb	1.31834	1.29067	1.26651	1.23879
53 s	-1.30299	-1.28108	-1.26146	-1.25068
54 pb	1.20814	1.18173	1.14714	1.11226
55 pb	1.20814	1.18173	1.14714	1.11226
56 s	-1.30299	-1.28108	-1.26146	-1.25068
57 pb	1.20814	1.18173	1.14714	1.11226
58 s	-1.30299	-1.28108	-1.26146	-1.25068
59 s	-1.30299	-1.28108	-1.26146	-1.25068
60 pb	1.20814	1.18173	1.14714	1.11226
61 s	-1.2235	-1.2048	-1.17672	-1.15631
62 pb	1.31834	1.29067	1.26651	1.23879
63 pb	1.31834	1.29067	1.26651	1.23879
64 s	-1.2235	-1.2048	-1.17672	-1.15631

Table S10 *BHLYP optimised structure for* $(MgO)_{32}$.

Mg	-1.0277312	3.0116526	3.0116526
O	0.9879546	3.0711083	3.0711083
O	-0.9966669	0.9966669	3.1235099
Mg	0.9975966	0.9975966	3.0921183
Mg	-0.9975966	-0.9975966	3.0921183
O	0.9966669	-0.9966669	3.1235099
O	-0.9879546	-3.0711083	3.0711083
Mg	1.0277312	-3.0116526	3.0116526
Mg	2.8864030	2.8864030	2.8864030
O	3.0711083	0.9879546	3.0711083
Mg	3.0116526	-1.0277312	3.0116526
O	2.9779056	-2.9779056	2.9779056
Mg	-2.8864030	-2.8864030	2.8864030
O	-3.0711083	-0.9879546	3.0711083
Mg	-3.0116526	1.0277312	3.0116526
O	-2.9779056	2.9779056	2.9779056
Mg	-3.0116526	3.0116526	1.0277312
O	-3.0711083	3.0711083	-0.9879546
O	-3.1235099	0.9966669	0.9966669
Mg	-3.0921183	0.9975966	-0.9975966
Mg	-3.0921183	-0.9975966	0.9975966
O	-3.1235099	-0.9966669	-0.9966669
O	-3.0711083	-3.0711083	0.9879546
Mg	-3.0116526	-3.0116526	-1.0277312
Mg	-2.8864030	2.8864030	-2.8864030
O	-3.0711083	0.9879546	-3.0711083
Mg	-3.0116526	-1.0277312	-3.0116526
O	-2.9779056	-2.9779056	-2.9779056
Mg	2.8864030	-2.8864030	-2.8864030
O	3.0711083	-0.9879546	-3.0711083
Mg	3.0116526	1.0277312	-3.0116526
O	2.9779056	2.9779056	-2.9779056
O	0.9879546	-3.0711083	-3.0711083
Mg	0.9975966	-0.9975966	-3.0921183
O	0.9966669	0.9966669	-3.1235099
Mg	1.0277312	3.0116526	-3.0116526
Mg	-1.0277312	-3.0116526	-3.0116526
O	-0.9966669	-0.9966669	-3.1235099
Mg	-0.9975966	0.9975966	-3.0921183
O	-0.9879546	3.0711083	-3.0711083
O	3.0711083	-3.0711083	-0.9879546
Mg	3.0921183	-0.9975966	-0.9975966
O	3.1235099	0.9966669	-0.9966669
Mg	3.0116526	3.0116526	-1.0277312
Mg	3.0116526	-3.0116526	1.0277312
O	3.1235099	-0.9966669	0.9966669
Mg	3.0921183	0.9975966	0.9975966
O	3.0711083	3.0711083	0.9879546
Mg	0.9975966	-3.0921183	-0.9975966
O	0.9966669	-3.1235099	0.9966669
O	-0.9966669	-3.1235099	-0.9966669
Mg	-0.9975966	-3.0921183	0.9975966
O	1.0219252	-1.0219252	-1.0219252
Mg	1.0214066	-1.0214066	1.0214066
Mg	-1.0214066	-1.0214066	-1.0214066
O	-1.0219252	-1.0219252	1.0219252
Mg	1.0214066	1.0214066	-1.0214066

O	1.0219252	1.0219252	1.0219252
O	-1.0219252	1.0219252	-1.0219252
Mg	-1.0214066	1.0214066	1.0214066
O	0.9966669	3.1235099	-0.9966669
Mg	0.9975966	3.0921183	0.9975966
Mg	-0.9975966	3.0921183	-0.9975966
O	-0.9966669	3.1235099	0.9966669

Table S11 *BHLYP optimised structure for* $(CaO)_{32}$.

Ca	-1.1730964	3.4970294	3.4970294
O	1.1930546	3.4770303	3.4770303
O	-1.1756354	1.1756354	3.5445770
Ca	1.1560595	1.1560595	3.5746546
Ca	-1.1560595	-1.1560595	3.5746546
O	1.1756354	-1.1756354	3.5445770
O	-1.1930546	-3.4770303	3.4770303
Ca	1.1730964	-3.4970294	3.4970294
Ca	3.3893111	3.3893111	3.3893111
O	3.4770303	1.1930546	3.4770303
Ca	3.4970294	-1.1730964	3.4970294
O	3.3670174	-3.3670174	3.3670174
Ca	-3.3893111	-3.3893111	3.3893111
O	-3.4770303	-1.1930546	3.4770303
Ca	-3.4970294	1.1730964	3.4970294
O	-3.3670174	3.3670174	3.3670174
Ca	-3.4970294	3.4970294	1.1730964
O	-3.4770303	3.4770303	-1.1930546
O	-3.5445770	1.1756354	1.1756354
Ca	-3.5746546	1.1560595	-1.1560595
Ca	-3.5746546	-1.1560595	1.1560595
O	-3.5445770	-1.1756354	-1.1756354
O	-3.4770303	-3.4770303	1.1930546
Ca	-3.4970294	-3.4970294	-1.1730964
Ca	-3.3893111	3.3893111	-3.3893111
O	-3.4770303	1.1930546	-3.4770303
Ca	-3.4970294	-1.1730964	-3.4970294
O	-3.3670174	-3.3670174	-3.3670174
Ca	3.3893111	-3.3893111	-3.3893111
O	3.4770303	-1.1930546	-3.4770303
Ca	3.4970294	1.1730964	-3.4970294
O	3.3670174	3.3670174	-3.3670174
O	1.1930546	-3.4770303	-3.4770303
Ca	1.1560595	-1.1560595	-3.5746546
O	1.1756354	1.1756354	-3.5445770
Ca	1.1730964	3.4970294	-3.4970294
Ca	-1.1730964	-3.4970294	-3.4970294
O	-1.1756354	-1.1756354	-3.5445770
Ca	-1.1560595	1.1560595	-3.5746546
O	-1.1930546	3.4770303	-3.4770303
O	3.4770303	-3.4770303	-1.1930546
Ca	3.5746546	-1.1560595	-1.1560595
O	3.5445770	1.1756354	-1.1756354
Ca	3.4970294	3.4970294	-1.1730964
Ca	3.4970294	-3.4970294	1.1730964
O	3.5445770	-1.1756354	1.1756354
Ca	3.5746546	1.1560595	1.1560595
O	3.4770303	3.4770303	1.1930546

Ca	1.1560595	-3.5746546	-1.1560595
O	1.1756354	-3.5445770	1.1756354
O	-1.1756354	-3.5445770	-1.1756354
Ca	-1.1560595	-3.5746546	1.1560595
O	1.1879863	-1.1879863	-1.1879863
Ca	1.1734556	-1.1734556	1.1734556
Ca	-1.1734556	-1.1734556	-1.1734556
O	-1.1879863	-1.1879863	1.1879863
Ca	1.1734556	1.1734556	-1.1734556
O	1.1879863	1.1879863	1.1879863
O	-1.1879863	1.1879863	-1.1879863
Ca	-1.1734556	1.1734556	1.1734556
O	1.1756354	3.5445770	-1.1756354
Ca	1.1560595	3.5746546	1.1560595
Ca	-1.1560595	3.5746546	-1.1560595
O	-1.1756354	3.5445770	1.1756354

Table S12 *BHLYP optimised structure for* $(SrO)_{32}$.

Sr	-1.2563008	3.7658826	3.7658826
O	1.3100490	3.6949401	3.6949401
O	-1.2855187	1.2855187	3.7830932
Sr	1.2405094	1.2405094	3.8472054
Sr	-1.2405094	-1.2405094	3.8472054
O	1.2855187	-1.2855187	3.7830932
O	-1.3100490	-3.6949401	3.6949401
Sr	1.2563008	-3.7658826	3.7658826
Sr	3.6542550	3.6542550	3.6542550
O	3.6949401	1.3100490	3.6949401
Sr	3.7658826	-1.2563008	3.7658826
O	3.5813948	-3.5813948	3.5813948
Sr	-3.6542550	-3.6542550	3.6542550
O	-3.6949401	-1.3100490	3.6949401
Sr	-3.7658826	1.2563008	3.7658826
O	-3.5813948	3.5813948	3.5813948
Sr	-3.7658826	3.7658826	1.2563008
O	-3.6949401	3.6949401	-1.3100490
O	-3.7830932	1.2855187	1.2855187
Sr	-3.8472054	1.2405094	-1.2405094
Sr	-3.8472054	-1.2405094	1.2405094
O	-3.7830932	-1.2855187	-1.2855187
O	-3.6949401	-3.6949401	1.3100490
Sr	-3.7658826	-3.7658826	-1.2563008
Sr	-3.6542550	3.6542550	-3.6542550
O	-3.6949401	1.3100490	-3.6949401
Sr	-3.7658826	-1.2563008	-3.7658826
O	-3.5813948	-3.5813948	-3.5813948
Sr	3.6542550	-3.6542550	-3.6542550
O	3.6949401	-1.3100490	-3.6949401
Sr	3.7658826	1.2563008	-3.7658826
O	3.5813948	3.5813948	-3.5813948
O	1.3100490	-3.6949401	-3.6949401
Sr	1.2405094	-1.2405094	-3.8472054
O	1.2855187	1.2855187	-3.7830932
Sr	1.2563008	3.7658826	-3.7658826
Sr	-1.2563008	-3.7658826	-3.7658826
O	-1.2855187	-1.2855187	-3.7830932

Sr	-1.2405094	1.2405094	-3.8472054
O	-1.3100490	3.6949401	-3.6949401
O	3.6949401	-3.6949401	-1.3100490
Sr	3.8472054	-1.2405094	-1.2405094
O	3.7830932	1.2855187	-1.2855187
Sr	3.7658826	3.7658826	-1.2563008
Sr	3.7658826	-3.7658826	1.2563008
O	3.7830932	-1.2855187	1.2855187
Sr	3.8472054	1.2405094	1.2405094
O	3.6949401	3.6949401	1.3100490
Sr	1.2405094	-3.8472054	-1.2405094
O	1.2855187	-3.7830932	1.2855187
O	-1.2855187	-3.7830932	-1.2855187
Sr	-1.2405094	-3.8472054	1.2405094
O	1.2869855	-1.2869855	-1.2869855
Sr	1.2628302	-1.2628302	1.2628302
Sr	-1.2628302	-1.2628302	-1.2628302
O	-1.2869855	-1.2869855	1.2869855
Sr	1.2628302	1.2628302	-1.2628302
O	1.2869855	1.2869855	1.2869855
O	-1.2869855	1.2869855	-1.2869855
Sr	-1.2628302	1.2628302	1.2628302
O	1.2855187	3.7830932	-1.2855187
Sr	1.2405094	3.8472054	1.2405094
Sr	-1.2405094	3.8472054	-1.2405094
O	-1.2855187	3.7830932	1.2855187

Table S13 *BHLYP optimised structure for* $(MgS)_{32}$.

Mg	-1.3424995	3.6592294	3.6592294
S	1.2006144	3.8887317	3.8887317
S	-1.2202980	1.2202980	3.9671802
Mg	1.3005829	1.3005829	3.7733457
Mg	-1.3005829	-1.3005829	3.7733457
S	1.2202980	-1.2202980	3.9671802
S	-1.2006144	-3.8887317	3.8887317
Mg	1.3424995	-3.6592294	3.6592294
Mg	3.4951385	3.4951385	3.4951385
S	3.8887317	1.2006144	3.8887317
Mg	3.6592294	-1.3424995	3.6592294
S	3.7786735	-3.7786735	3.7786735
Mg	-3.4951385	-3.4951385	3.4951385
S	-3.8887317	-1.2006144	3.8887317
Mg	-3.6592294	1.3424995	3.6592294
S	-3.7786735	3.7786735	3.7786735
Mg	-3.6592294	3.6592294	1.3424995
S	-3.8887317	3.8887317	-1.2006144
S	-3.9671802	1.2202980	1.2202980
Mg	-3.7733457	1.3005829	-1.3005829
Mg	-3.7733457	-1.3005829	1.3005829
S	-3.9671802	-1.2202980	-1.2202980
S	-3.8887317	-3.8887317	1.2006144
Mg	-3.6592294	-3.6592294	-1.3424995
Mg	-3.4951385	3.4951385	-3.4951385
S	-3.8887317	1.2006144	-3.8887317
Mg	-3.6592294	-1.3424995	-3.6592294
S	-3.7786735	-3.7786735	-3.7786735

Mg	3.4951385	-3.4951385	-3.4951385
S	3.8887317	-1.2006144	-3.8887317
Mg	3.6592294	1.3424995	-3.6592294
S	3.7786735	3.7786735	-3.7786735
S	1.2006144	-3.8887317	-3.8887317
Mg	1.3005829	-1.3005829	-3.7733457
S	1.2202980	1.2202980	-3.9671802
Mg	1.3424995	3.6592294	-3.6592294
Mg	-1.3424995	-3.6592294	-3.6592294
S	-1.2202980	-1.2202980	-3.9671802
Mg	-1.3005829	1.3005829	-3.7733457
S	-1.2006144	3.8887317	-3.8887317
S	3.8887317	-3.8887317	-1.2006144
Mg	3.7733457	-1.3005829	-1.3005829
S	3.9671802	1.2202980	-1.2202980
Mg	3.6592294	3.6592294	-1.3424995
Mg	3.6592294	-3.6592294	1.3424995
S	3.9671802	-1.2202980	1.2202980
Mg	3.7733457	1.3005829	1.3005829
S	3.8887317	3.8887317	1.2006144
Mg	1.3005829	-3.7733457	-1.3005829
S	1.2202980	-3.9671802	1.2202980
S	-1.2202980	-3.9671802	-1.2202980
Mg	-1.3005829	-3.7733457	1.3005829
S	1.2564784	-1.2564784	-1.2564784
Mg	1.3085941	-1.3085941	1.3085941
Mg	-1.3085941	-1.3085941	-1.3085941
S	-1.2564784	-1.2564784	1.2564784
Mg	1.3085941	1.3085941	-1.3085941
S	1.2564784	1.2564784	1.2564784
S	-1.2564784	1.2564784	-1.2564784
Mg	-1.3085941	1.3085941	1.3085941
S	1.2202980	3.9671802	-1.2202980
Mg	1.3005829	3.7733457	1.3005829
Mg	-1.3005829	3.7733457	-1.3005829
S	-1.2202980	3.9671802	1.2202980

Table S14 *BHLYP Optimised structure for* $(MgSe)_{32}$.

Mg	-1.4353564	3.8317213	3.8317213
Se	1.2585890	4.1162969	4.1162969
Se	-1.2781548	1.2781548	4.2064929
Mg	1.3945905	1.3945905	3.9554740
Mg	-1.3945905	-1.3945905	3.9554740
Se	1.2781548	-1.2781548	4.2064929
Se	-1.2585890	-4.1162969	4.1162969
Mg	1.4353564	-3.8317213	3.8317213
Mg	3.6580732	3.6580732	3.6580732
Se	4.1162969	1.2585890	4.1162969
Mg	3.8317213	-1.4353564	3.8317213
Se	4.0010859	-4.0010859	4.0010859
Mg	-3.6580732	-3.6580732	3.6580732
Se	-4.1162969	-1.2585890	4.1162969
Mg	-3.8317213	1.4353564	3.8317213
Se	-4.0010859	4.0010859	4.0010859
Mg	-3.8317213	3.8317213	1.4353564
Se	-4.1162969	4.1162969	-1.2585890

Se	-4.2064929	1.2781548	1.2781548
Mg	-3.9554740	1.3945905	-1.3945905
Mg	-3.9554740	-1.3945905	1.3945905
Se	-4.2064929	-1.2781548	-1.2781548
Se	-4.1162969	-4.1162969	1.2585890
Mg	-3.8317213	-3.8317213	-1.4353564
Mg	-3.6580732	3.6580732	-3.6580732
Se	-4.1162969	1.2585890	-4.1162969
Mg	-3.8317213	-1.4353564	-3.8317213
Se	-4.0010859	-4.0010859	-4.0010859
Mg	3.6580732	-3.6580732	-3.6580732
Se	4.1162969	-1.2585890	-4.1162969
Mg	3.8317213	1.4353564	-3.8317213
Se	4.0010859	4.0010859	-4.0010859
Se	1.2585890	-4.1162969	-4.1162969
Mg	1.3945905	-1.3945905	-3.9554740
Se	1.2781548	1.2781548	-4.2064929
Mg	1.4353564	3.8317213	-3.8317213
Mg	-1.4353564	-3.8317213	-3.8317213
Se	-1.2781548	-1.2781548	-4.2064929
Mg	-1.3945905	1.3945905	-3.9554740
Se	-1.2585890	4.1162969	-4.1162969
Se	4.1162969	-4.1162969	-1.2585890
Mg	3.9554740	-1.3945905	-1.3945905
Se	4.2064929	1.2781548	-1.2781548
Mg	3.8317213	3.8317213	-1.4353564
Mg	3.8317213	-3.8317213	1.4353564
Se	4.2064929	-1.2781548	1.2781548
Mg	3.9554740	1.3945905	1.3945905
Se	4.1162969	4.1162969	1.2585890
Mg	1.3945905	-3.9554740	-1.3945905
Se	1.2781548	-4.2064929	1.2781548
Se	-1.2781548	-4.2064929	-1.2781548
Mg	-1.3945905	-3.9554740	1.3945905
Se	1.3151707	-1.3151707	-1.3151707
Mg	1.4014159	-1.4014159	1.4014159
Mg	-1.4014159	-1.4014159	-1.4014159
Se	-1.3151707	-1.3151707	1.3151707
Mg	1.4014159	1.4014159	-1.4014159
Se	1.3151707	1.3151707	1.3151707
Se	-1.3151707	1.3151707	-1.3151707
Mg	-1.4014159	1.4014159	1.4014159
Se	1.2781548	4.2064929	-1.2781548
Mg	1.3945905	3.9554740	1.3945905
Mg	-1.3945905	3.9554740	-1.3945905
Se	-1.2781548	4.2064929	1.2781548

Table S15 *BHLYP optimised structure for* $(CdO)_{32}$.

Cd	-1.1313432	-3.4130673	-3.4130673
O	1.0869686	-3.4290084	-3.4290084
O	-1.1196131	-1.1196131	-3.5120904
Cd	1.1126827	-1.1126827	-3.5227343
Cd	-1.1126827	1.1126827	-3.5227343
O	1.1196131	1.1196131	-3.5120904
O	-1.0869686	3.4290084	-3.4290084
Cd	1.1313432	3.4130673	-3.4130673
Cd	3.2382884	-3.2382884	-3.2382884

O	3.4290084	-1.0869686	-3.4290084
Cd	3.4130673	1.1313432	-3.4130673
O	3.2804441	3.2804441	-3.2804441
Cd	-3.2382884	3.2382884	-3.2382884
O	-3.4290084	1.0869686	-3.4290084
Cd	-3.4130673	-1.1313432	-3.4130673
O	-3.2804441	-3.2804441	-3.2804441
Cd	-3.4130673	-3.4130673	-1.1313432
O	-3.4290084	-3.4290084	1.0869686
O	-3.5120904	-1.1196131	-1.1196131
Cd	-3.5227343	-1.1126827	1.1126827
Cd	-3.5227343	1.1126827	-1.1126827
O	-3.5120904	1.1196131	1.1196131
O	-3.4290084	3.4290084	-1.0869686
Cd	-3.4130673	3.4130673	1.1313432
Cd	-3.2382884	-3.2382884	3.2382884
O	-3.4290084	-1.0869686	3.4290084
Cd	-3.4130673	1.1313432	3.4130673
O	-3.2804441	3.2804441	3.2804441
Cd	3.2382884	3.2382884	3.2382884
O	3.4290084	1.0869686	3.4290084
Cd	3.4130673	-1.1313432	3.4130673
O	3.2804441	-3.2804441	3.2804441
O	1.0869686	3.4290084	3.4290084
Cd	1.1126827	1.1126827	3.5227343
O	1.1196131	-1.1196131	3.5120904
Cd	1.1313432	-3.4130673	3.4130673
Cd	-1.1313432	3.4130673	3.4130673
O	-1.1196131	1.1196131	3.5120904
Cd	-1.1126827	-1.1126827	3.5227343
O	-1.0869686	-3.4290084	3.4290084
O	3.4290084	3.4290084	1.0869686
Cd	3.5227343	1.1126827	1.1126827
O	3.5120904	-1.1196131	1.1196131
Cd	3.4130673	-3.4130673	1.1313432
Cd	3.4130673	3.4130673	-1.1313432
O	3.5120904	1.1196131	-1.1196131
Cd	3.5227343	-1.1126827	-1.1126827
O	3.4290084	-3.4290084	-1.0869686
Cd	1.1126827	3.5227343	1.1126827
O	1.1196131	3.5120904	-1.1196131
O	-1.1196131	3.5120904	1.1196131
Cd	-1.1126827	3.5227343	-1.1126827
O	1.1633164	1.1633164	1.1633164
Cd	1.1451857	1.1451857	-1.1451857
Cd	-1.1451857	1.1451857	1.1451857
O	-1.1633164	1.1633164	-1.1633164
Cd	1.1451857	-1.1451857	1.1451857
O	1.1633164	-1.1633164	-1.1633164
O	-1.1633164	-1.1633164	1.1633164
Cd	-1.1451857	-1.1451857	-1.1451857
O	1.1196131	-3.5120904	1.1196131
Cd	1.1126827	-3.5227343	-1.1126827
Cd	-1.1126827	-3.5227343	1.1126827
O	-1.1196131	-3.5120904	-1.1196131

Table S16 *BHLYP Optimised structure for* $(PbS)_{32}$.

Pb	-1.7937790	-4.5123516	-4.5123516
S	1.7852788	-4.5005900	-4.5005900
S	-1.7797764	-1.7797764	-4.4934626
Pb	1.7650475	-1.7650475	-4.5640431
Pb	-1.7650475	1.7650475	-4.5640431
S	1.7797764	1.7797764	-4.4934626
S	-1.7852788	4.5005900	-4.5005900
Pb	1.7937790	4.5123516	-4.5123516
Pb	4.4801322	-4.4801322	-4.4801322
S	4.5005900	-1.7852788	-4.5005900
Pb	4.5123516	1.7937790	-4.5123516
S	4.4942644	4.4942644	-4.4942644
Pb	-4.4801322	4.4801322	-4.4801322
S	-4.5005900	1.7852788	-4.5005900
Pb	-4.5123516	-1.7937790	-4.5123516
S	-4.4942644	-4.4942644	-4.4942644
Pb	-4.5123516	-4.5123516	-1.7937790
S	-4.5005900	-4.5005900	1.7852788
S	-4.4934626	-1.7797764	-1.7797764
Pb	-4.5640431	-1.7650475	1.7650475
Pb	-4.5640431	1.7650475	-1.7650475
S	-4.4934626	1.7797764	1.7797764
S	-4.5005900	4.5005900	-1.7852788
Pb	-4.5123516	4.5123516	1.7937790
Pb	-4.4801322	-4.4801322	4.4801322
S	-4.5005900	-1.7852788	4.5005900
Pb	-4.5123516	1.7937790	4.5123516
S	-4.4942644	4.4942644	4.4942644
Pb	4.4801322	4.4801322	4.4801322
S	4.5005900	1.7852788	4.5005900
Pb	4.5123516	-1.7937790	4.5123516
S	4.4942644	-4.4942644	4.4942644
S	1.7852788	4.5005900	4.5005900
Pb	1.7650475	1.7650475	4.5640431
S	1.7797764	-1.7797764	4.4934626
Pb	1.7937790	-4.5123516	4.5123516
Pb	-1.7937790	4.5123516	4.5123516
S	-1.7797764	1.7797764	4.4934626
Pb	-1.7650475	-1.7650475	4.5640431
S	-1.7852788	-4.5005900	4.5005900
S	4.5005900	4.5005900	1.7852788
Pb	4.5640431	1.7650475	1.7650475
S	4.4934626	-1.7797764	1.7797764
Pb	4.5123516	-4.5123516	1.7937790
Pb	4.5123516	4.5123516	-1.7937790
S	4.4934626	1.7797764	-1.7797764
Pb	4.5640431	-1.7650475	-1.7650475
S	4.5005900	-4.5005900	-1.7852788
Pb	1.7650475	4.5640431	1.7650475
S	1.7797764	4.4934626	-1.7797764
S	-1.7797764	4.4934626	1.7797764
Pb	-1.7650475	4.5640431	-1.7650475
S	1.7900869	1.7900869	1.7900869
Pb	1.7205072	1.7205072	-1.7205072
Pb	-1.7205072	1.7205072	1.7205072
S	-1.7900869	1.7900869	-1.7900869
Pb	1.7205072	-1.7205072	1.7205072

S	1.7900869	-1.7900869	-1.7900869
S	-1.7900869	-1.7900869	1.7900869
Pb	-1.7205072	-1.7205072	-1.7205072
S	1.7797764	-4.4934626	1.7797764
Pb	1.7650475	-4.5640431	-1.7650475
Pb	-1.7650475	-4.5640431	1.7650475
S	-1.7797764	-4.4934626	-1.7797764