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Supporting Information for chemical communications

Functionalized Deltahedral Zintl Complex Ge_9R_3 (R = CF_3, CN, NO_2): A New Class of Superhalogen

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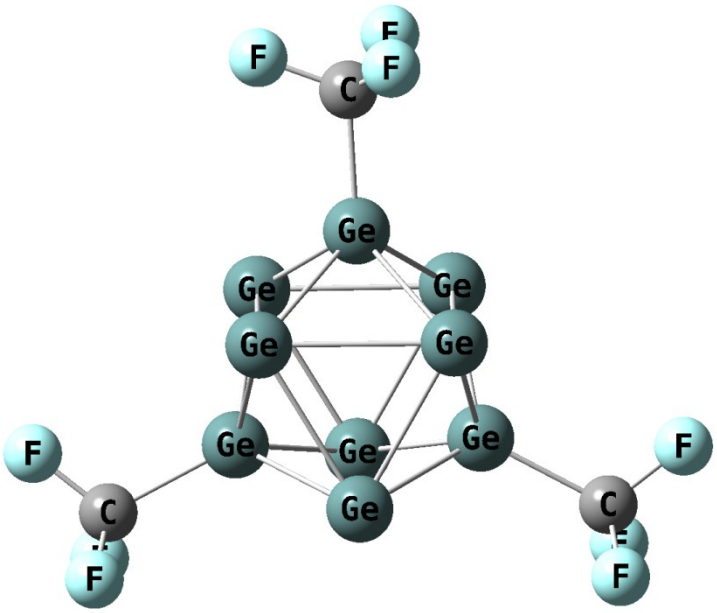
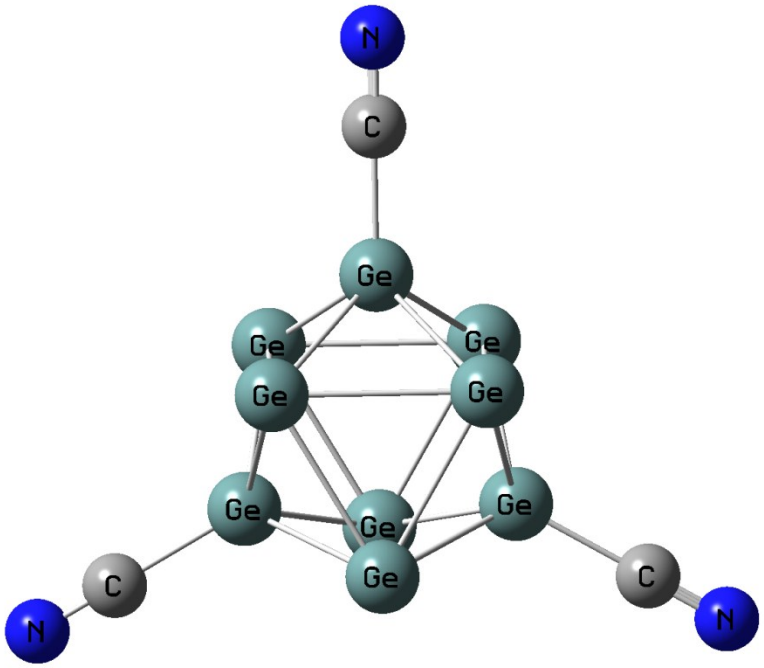
Figure S1. Optimized geometry and cartesian coordinates of $[Ge_9(CF_3)_3]^-$ are given below.



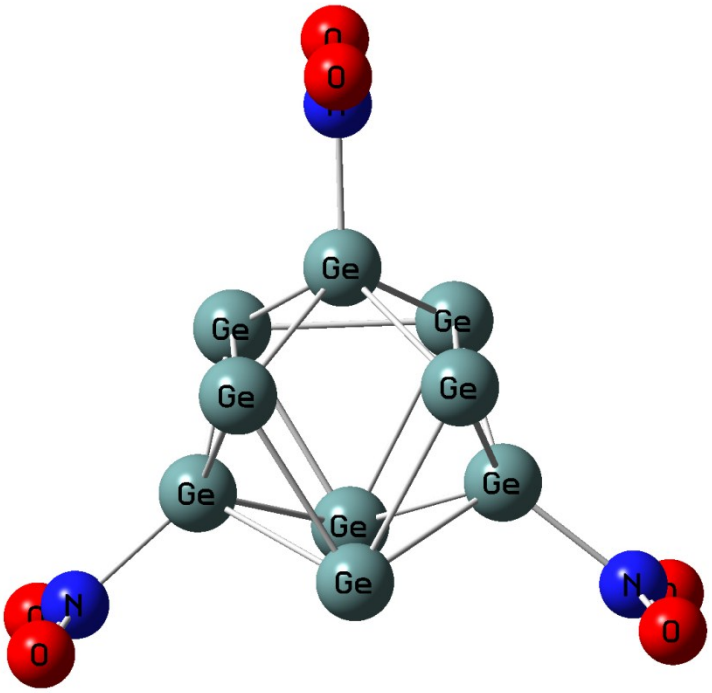
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	0.472275	-1.546000	1.715095
2	32	0	1.932575	-0.406866	0.008177
3	32	0	0.491396	-1.542562	-1.714229
4	32	0	-1.519240	0.336857	1.793765
5	32	0	-0.611124	1.847786	-0.002120
6	32	0	-1.503631	0.340306	-1.808622
7	32	0	1.085188	1.167757	-1.747337
8	32	0	1.068434	1.168134	1.756996
9	32	0	-1.363756	-1.404881	-0.007597
10	6	0	3.868772	-0.838115	0.005561
11	6	0	-1.208809	3.739047	0.000576
12	6	0	-2.706926	-2.865784	-0.001911
13	9	0	4.660079	0.272420	0.113439
14	9	0	4.268047	-1.473323	-1.136839
15	9	0	4.231049	-1.655035	1.040082
16	9	0	-3.990130	-2.405310	-0.116337
17	9	0	-2.537120	-3.749915	-1.030993
18	9	0	-2.677603	-3.608740	1.145164
19	9	0	-2.570229	3.869650	-0.038422
20	9	0	-0.800955	4.421609	1.112856
21	9	0	-0.737132	4.445546	-1.070891

Figure S2. Optimized geometry and cartesian coordinates of $[Ge_9(CN)_3]^-$ are given below.



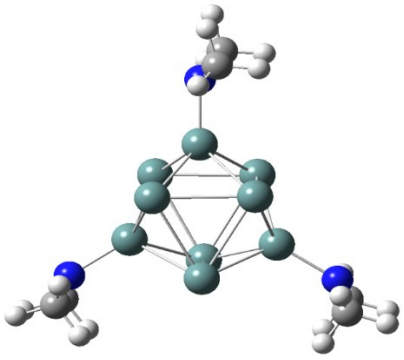
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	0.993007	1.246808	-1.810379
2	32	0	1.988980	-0.298704	0.000585
3	32	0	0.993768	1.247267	1.810754
4	32	0	-1.576209	0.237038	-1.810445
5	32	0	-1.252581	-1.573627	0.000359
6	32	0	-1.577419	0.236650	1.810538
7	32	0	0.583377	-1.483935	1.811054
8	32	0	0.582971	-1.482282	-1.811464
9	32	0	-0.735889	1.871242	0.000883
10	6	0	-1.443478	3.674578	-0.000762
11	6	0	3.904514	-0.587935	-0.001264
12	6	0	-2.460946	-3.087685	-0.001581
13	7	0	-1.865718	4.751189	-0.001334
14	7	0	5.047961	-0.760849	-0.001866
15	7	0	-3.182348	-3.991538	-0.002319

Figure S3. Optimized geometry and cartesian coordinates of $[Ge_9(NO_2)_3]^-$ are given below.



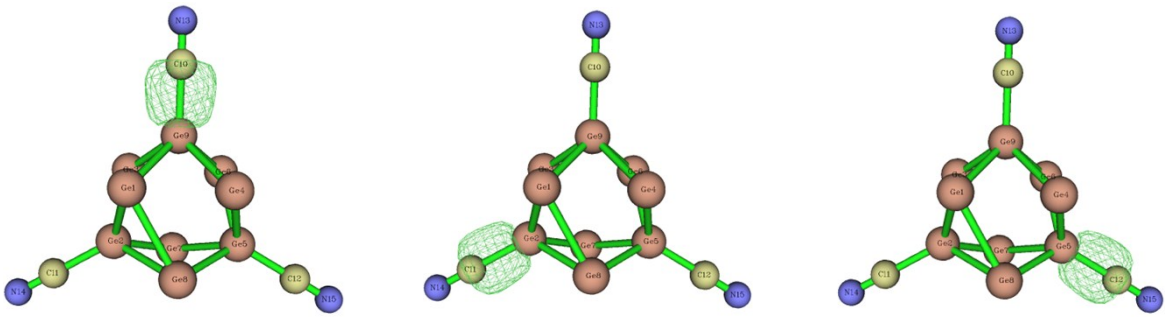
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	-0.806268	1.352816	-1.926123
2	32	0	0.819319	1.845917	-0.000000
3	32	0	-0.805769	1.352596	1.926486
4	32	0	-0.811718	-1.342334	-1.938394
5	32	0	0.799442	-1.860050	-0.000208
6	32	0	-0.811217	-1.342560	1.938451
7	32	0	1.629424	-0.008318	1.626070
8	32	0	1.628995	-0.008134	-1.626495
9	32	0	-1.933809	-0.002831	0.000252
10	8	0	-4.543096	-0.014853	1.080571
11	8	0	2.517654	-3.821252	1.079735
12	8	0	2.475956	3.855994	1.080233
13	7	0	2.149638	-3.379448	-0.000466
14	7	0	-3.966031	-0.012097	0.000490
15	7	0	2.120620	3.404657	-0.000064
16	8	0	2.517368	-3.821167	-1.080804
17	8	0	2.475667	3.856143	-1.080395
18	8	0	-4.543345	-0.014753	-1.079455

Figure S4. Optimized geometry and cartesian coordinates of $[Ge_9(NO_2)_3]^-$ are given below.



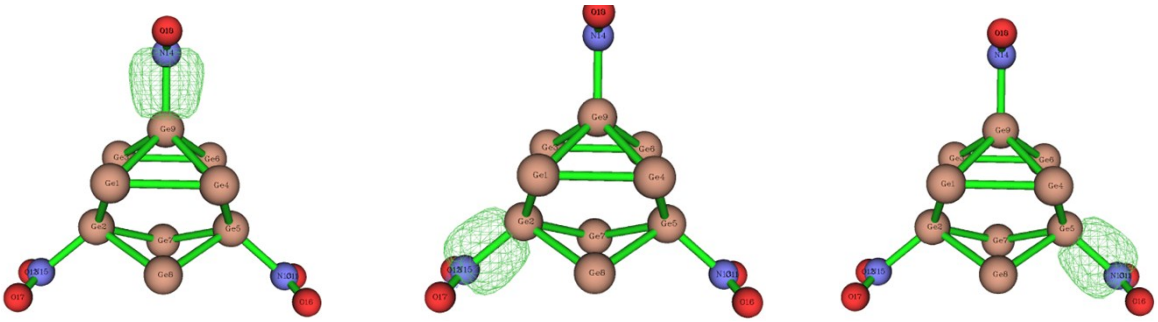
VDE = 2.47 eV

Center Number	Coordinates (Angstroms) X	Y	Z
1	1.594134	0.318869	1.562362
2	0.430129	2.050608	0.024119
3	1.588743	0.356766	-1.564603
4	-0.472965	-1.502273	1.914858
5	-1.960023	-0.589623	-0.008693
6	-0.480477	-1.447484	-1.968242
7	-1.119438	1.150863	-1.789734
8	-1.115207	1.109748	1.812369
9	1.192008	-1.726288	-0.030391
10	1.077070	3.835032	0.042156
11	-3.820091	-1.019034	-0.013566
12	2.594410	-3.010818	-0.043620
13	-4.536082	-0.723326	1.210126
14	-5.514607	-1.222386	1.197081
15	-3.984649	-1.097726	2.073574
16	-4.717966	0.353613	1.372816
17	-4.558276	-0.607969	-1.189833
18	-4.025876	-0.901994	-2.095211
19	-5.538838	-1.102932	-1.203829
20	-4.737520	0.480066	-1.247402
21	3.495966	-2.978003	-1.176383
22	4.070105	-3.913465	-1.220880
23	2.934551	-2.888194	-2.107042
24	4.221173	-2.146811	-1.143107
25	3.293352	-3.201965	1.210271
26	3.863347	-4.140364	1.178771
27	4.003325	-2.391971	1.450823
28	2.581882	-3.271693	2.034258
29	1.776894	4.274012	-1.148071
30	1.224496	3.982565	-2.042081
31	1.857899	5.369208	-1.146526
32	2.798597	3.867551	-1.239923
33	1.737214	4.260878	1.259504
34	2.755863	3.854138	1.379765
35	1.816875	5.356066	1.273411
36	1.156291	3.958335	2.131561



2c-2e ON = 1.99 |e| 2c-2e ON = 1.99 |e| 2c-2e ON = 1.99 |e|

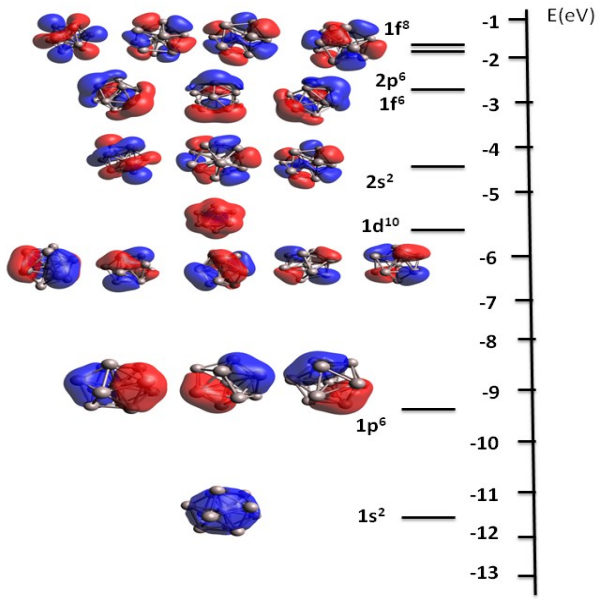
$[Ge_9(CN)_3]^-$



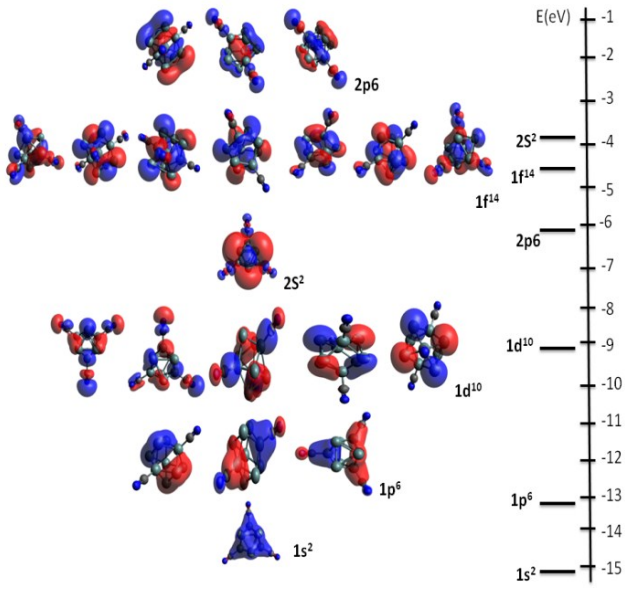
2c-2e ON = 1.99 |e| 2c-2e ON = 1.99 |e| 2c-2e ON = 1.99 |e|

$[Ge_9(NO_2)_3]^-$

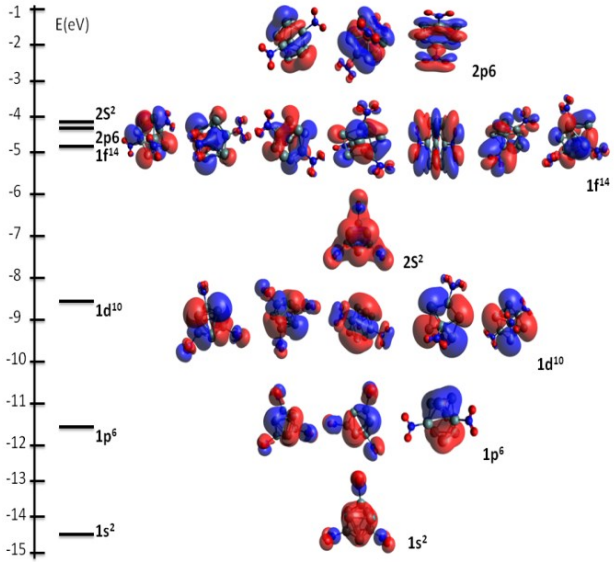
Figure S5. AdNDP localization results of $[Ge_9(CN)_3]^-$ and $[Ge_9(NO_2)_3]^-$ with occupation numbers.



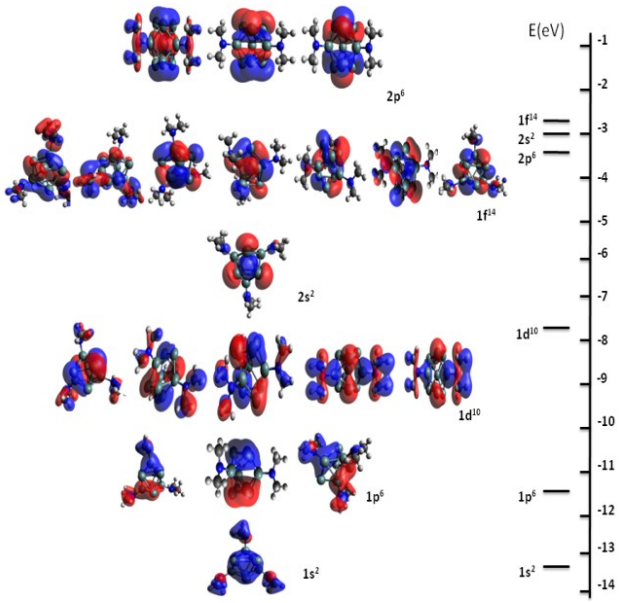
Al_{13}^-



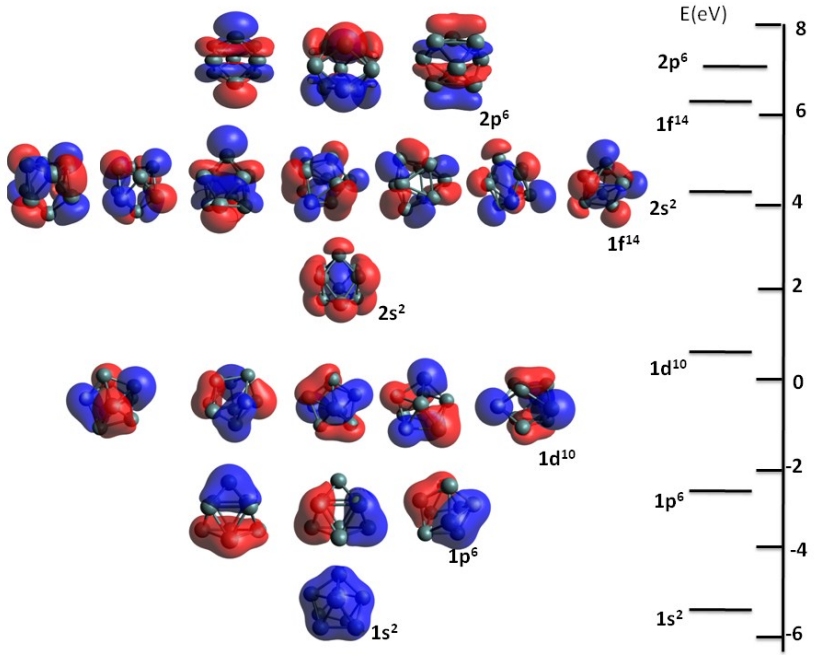
$[Ge_9(CN)_3]^-$



$[Ge_9(NO_2)_3]^-$

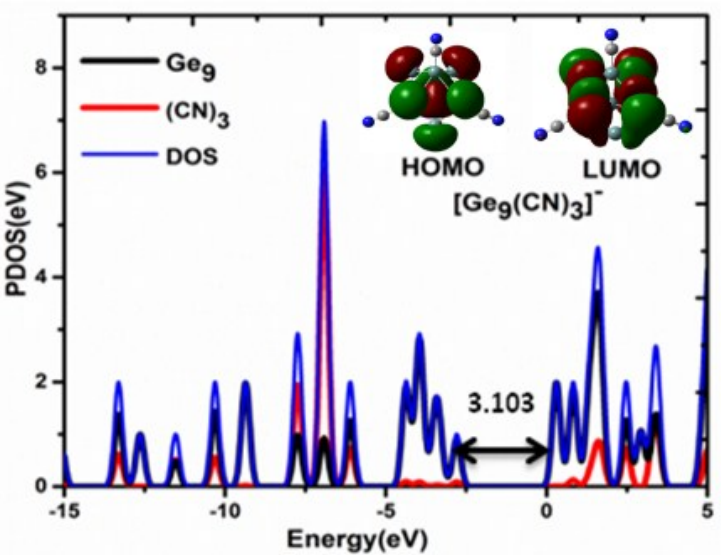


$[Ge_9(NMe_2)_3]^-$



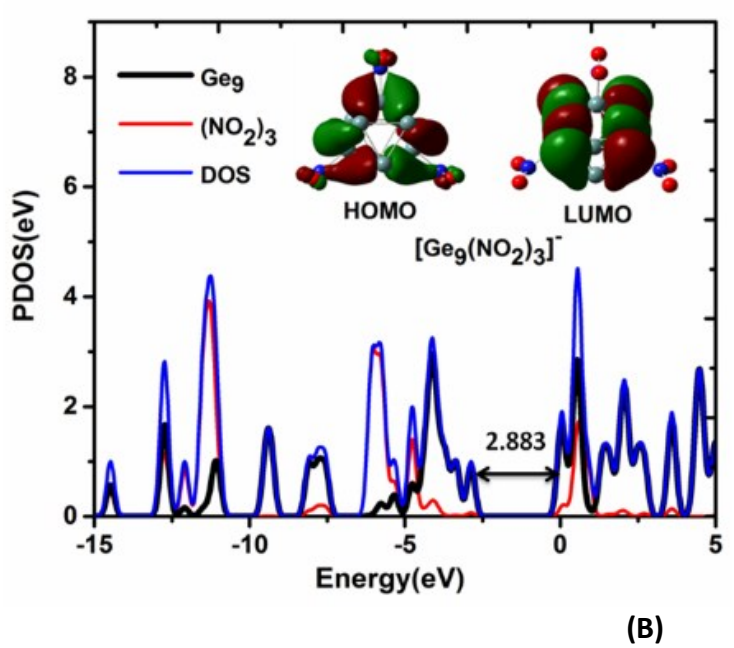
Ge_9^{4-}

Figure S6. Molecular orbitals of Al_{13}^-, $[Ge_9(CN)_3]^-$, $[Ge_9(NO_2)_3]^-$,$[Ge_9(NMe_2)_3]^-$ and Ge_9^{4-}



	Ge	$(CN)_3$	
LUMO+4	100	0	
LUMO +3	94	6	
LUMO+2	94	6	
LUMO+1	100	0	
LUMO	100	0	
HOMO	91	9	
HOMO -1	98	2	
HOMO -2	99	1	
HOMO -3	97	3	
HOMO -4	97	3	
HOMO -5	97	3	
HOMO -6	95	5	
HOMO -7	95	5	
HOMO -8	63	37	
HOMO -9	63	37	

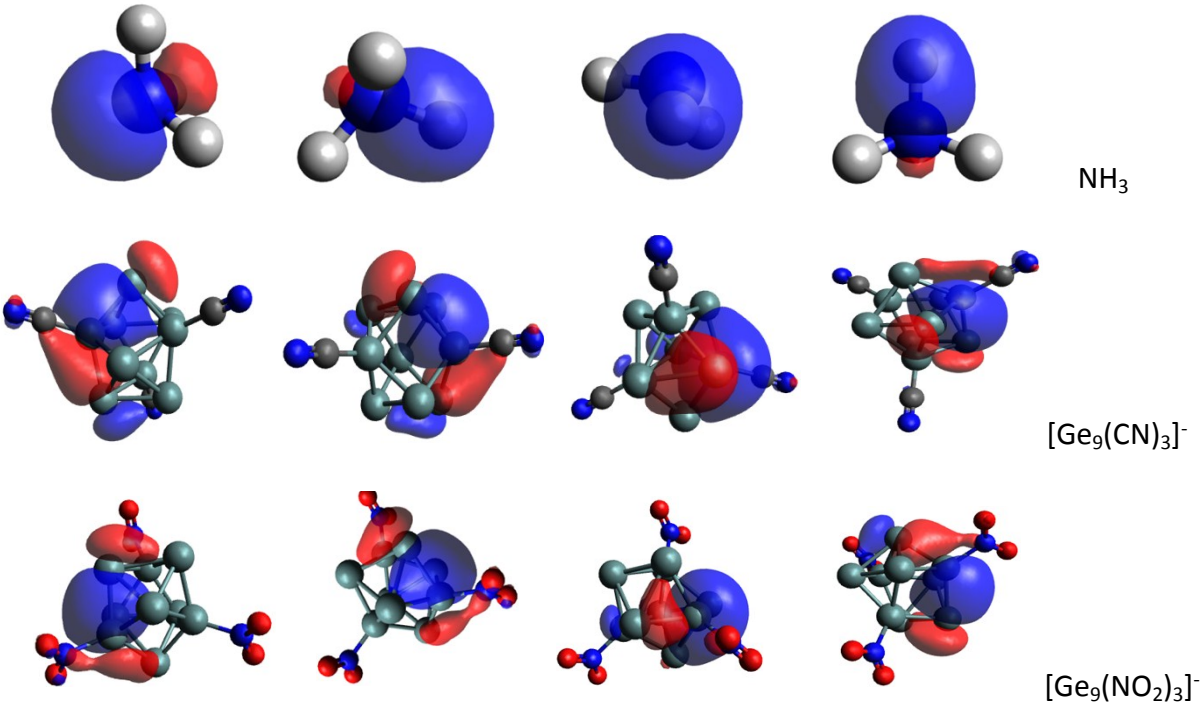
(A)

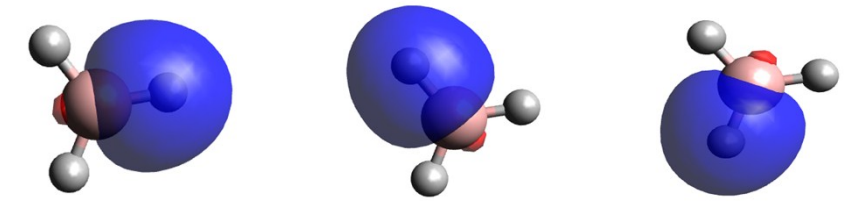


(B)

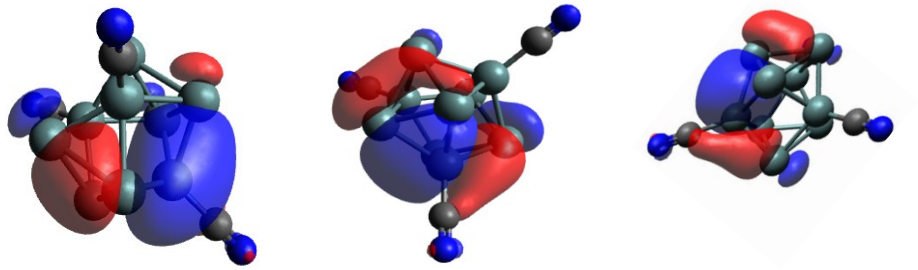
	Ge	$(NO_2)_3$
LUMO+4	100	0
LUMO +3	91	9
LUMO+2	77	23
LUMO+1	80	20
LUMO	100	0
HOMO	93	7
HOMO -1	98	2
HOMO -2	99	1
HOMO -3	92	8
HOMO -4	84	16
HOMO -5	97	3
HOMO -6	92	8
HOMO -7	89	11
HOMO -8	31	69
HOMO -9	28	72

Figure S7: The calculated PDOS diagrams and contribution of core and ligand toward FMO of (A) $[Ge_9(CN)_3]^-$ and (B) $[Ge_9(NO_2)_3]^-$; Black, Red and Blue color indicates Ge_9 core, ligands (CN, NO_2) and total DOS respectively.

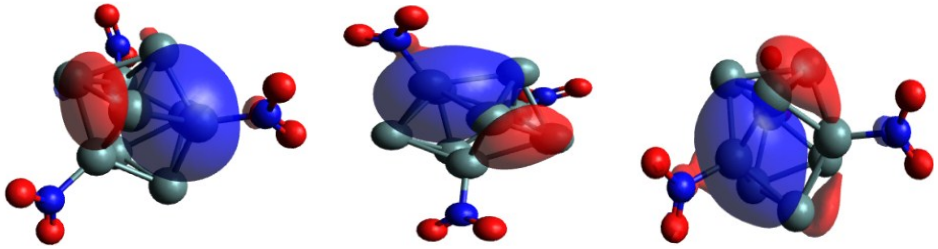




BH_3



$[Ge_9(CN)_3]$



$[Ge_9(NO_2)_3]$

Figure S8. Comparison of Natural Localized molecular orbitals (NLMO's) for proposed $[Ge_9(CN)_3]^-$, $[Ge_9(NO_2)_3]^-$, $[Ge_9(CN)_3]$, $[Ge_9(NO_2)_3]$ clusters and NH_3 , BH_3 molecules .