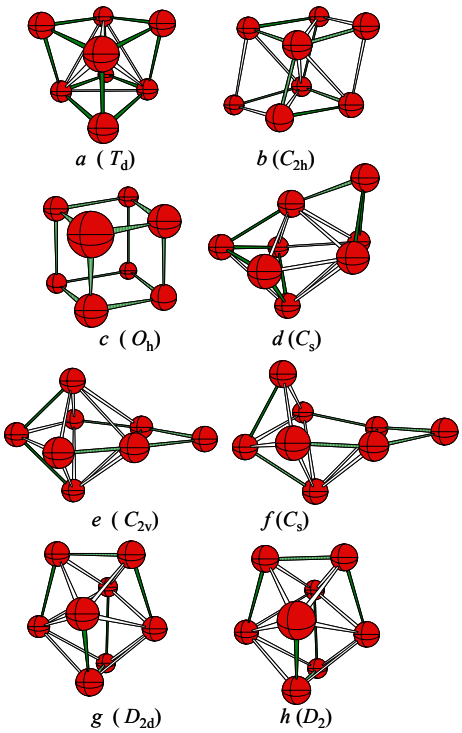
S-Table 1. B3LYP/6-31G* total energies (au), zero-point energies (ZPE, kcal/mol) and relative energies (with ZPE, kcal/mol) as well as MP2 total energies and relative energies for selective species.

Species	Symm.	E_{tot}(B3LYP)	ZPE (B3LYP)	E_{rel} (+ZPE)	E_{tot}(MP2)	E_{rel} (MP2+ZPE)
1 ($C_{10}H_{12}^{2+}$)	T_d	-387.50975	122.8			
2 ($C_6Si_4H_{12}^{2+}$)	T_d	-1393.26436	105.9			
3 ($C_6Ge_4H_{12}^{2+}$)	T_d	-8535.31823	104.5			
4 ($C_8H_4^{2+}$)	T_d	-306.07727	51.9			
5 ($C_4Si_4H_4^{2+}$)	T_d	-1311.99446	42.3			
6 ($Si_8H_4^{2+}$)	T_d	-2317.63864	27.0			
7 ($Ge_8H_4^{2+}$)	T_d	-16601.96694	23.9			
8 (C_8^{2-})	T_d	-304.17150	19.8			
9 (Si_8^{2-})	T_d	-2315.92437	7.7			
10 (Ge_8^{2-})	T_d	-16600.23928	4.7			
11 (Si_8Li_2)	C_s	-2331.02089	10.0			
12 (Si_8Li^-)	C_{2v}	-2323.54017	9.0			
13 (Si_8Na_2)	C_s	-2640.55579	8.8			
14 (Si_8Na^-)	C_{2v}	-2478.30047	8.4			
15 (Ge_8Li_2)	C_s	-16615.40115	7.2			
16 (Ge_8Li^-)	C_{2v}	-16607.89148	6.1			
17 (Ge_8Na_2)	C_s	-16924.92855	5.8			
18 (Ge_8Na^-)	C_{2v}	-16762.64771	5.3			
19 (C_8H_2)	C_s	-305.53289	37.0			
20 (Si_8H_2)	C_s	-2317.08149	17.3			
21 (Ge_8H_2)	C_s	-16601.40044	14.1			
22 ($C_{20}H_{12}$)	T_h (nonet)	-768.85411	157.3	-4.8	-766.39596	82.9
	T_h	-768.84646	157.3	0.0	-766.52806	0.0
23 ($C_{12}Si_8H_{12}$)	T_h (nonet)	-2780.17895	131.9	53.3		
	T_h	-2780.26380	131.9	0.0		
24 ($C_{12}Ge_8H_{12}$)	T_h (nonet)	-17064.32320	128.3	91.3		
	T_h	-17064.46964	128.8	0.0		
25 ($C_{20}H_{24}$)	T_h (nonet)	-776.14501	240.6	-3.2	-773.44425	70.4
	T_h	-776.13884	239.8	0.0	-773.55530	0.0
	D_{2d}	-776.45225	248.2	-188.3		
	D_{4h}	-776.46245	247.6	-195.3		
Ni@**25**	T_h	-2284.45541	242.4			
26 ($C_{12}Si_8H_{24}$)	T_h (nonet)	-2787.44027	208.2	66.5		
	T_h	-2787.53845	203.3	0.0		
	D_{2d}	-2787.66046	206.4	-73.4		
Ni@**26**	T_h	-4295.94803	207.3			
27 ($C_{12}Ge_8H_{24}$)	T_h (nonet)	-17071.52982	206.0	101.2		
	T_h	-17071.67971	198.9	0.0		

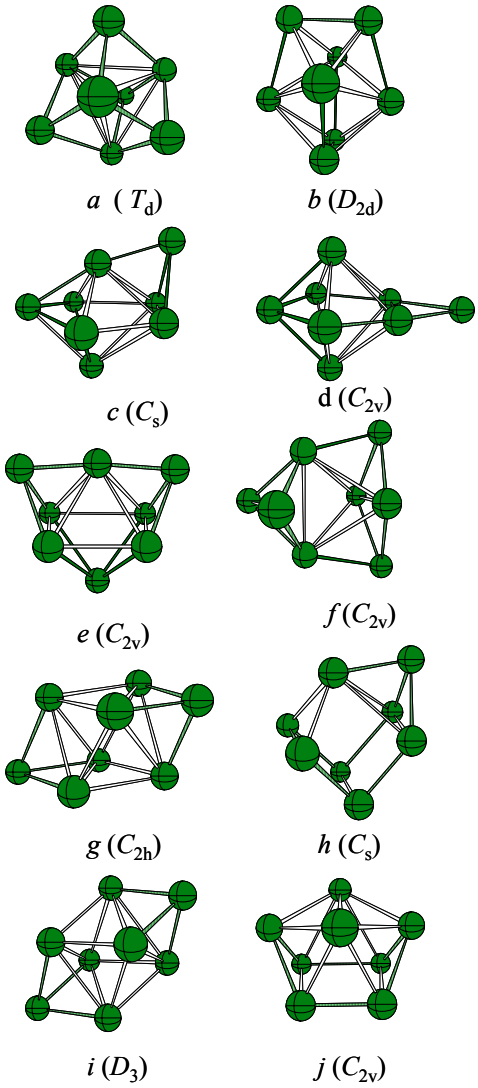
	D_{2d}	-17071.80521	202.4	-75.3
Ni@**27**	T_h	-18580.13248	201.1	
28 ($C_{10}H_4^{4+}$)	T_d	-380.44549	51.7	
29 ($C_4Si_6H_4^{4+}$)	T_d	-1889.68693	42.9	
30 ($C_4Ge_6H_4^{4+}$)	T_d	-12602.88550	40.2	
31 ($Si_{10}H_4^{4+}$)	T_d	-2895.37233	27.7	
32 ($Ge_{10}H_4^{4+}$)	T_d	-20750.78954	22.1	
33 ($C_6Bi_4H_4$)	T_d	-330.040103	48.3	
34 ($Si_6Bi_4H_4$)	T_d	-1838.68383	37.6	
35 ($Ge_6Bi_4H_4$)	T_d	-12551.91779	36.4	

S-Table 2. Total energies(au), relative energies, zero-point energies (kcal/mol),relative energies (with ZPE, kcal/mol), number of imaginary frequencies and mode following converged local minima structures, and HOMO-LUMO gap energies of X_8^{2-}(X= Si and Ge) isomers (see S-Figure 1and S-Figure 2)

Species	Symm.	E_{tot}	ZPE	E_{rel}(+ZPE)	NIMAG	Gap
Si_8^{2-}	a (T_d)	-2315.92437	7.7	0.0	0	3.25
	b (C_{2h})	-2315.87291	7.0	31.6	0	1.84
	c (O_h)	-2315.88359	7.1	25.0	1–> a (T_d)	2.74
	d (C_s)	-2315.88473	6.6	23.8	0	2.24
	e (C_{2v})	-2315.85806	6.3	40.2	1–> f (C_s)	2.07
	f (C_s)	-2315.85874	6.5	40.0	0	1.86
	g (D_{2d})	-2315.88948	6.5	20.7	1–> h (D_2)	2.15
	h (D_2)	-2315.8900	6.7	20.6	0	2.10
Ge_8^{2-}	a (T_d)	-16600.23928	4.7	0.0	0	3.19
	b (D_{2d})	-16600.21211	4.0	16.3	0	2.20
	c (C_s)	-16600.20085	4.0	23.4	0	2.17
	d (C_{2v})	-16600.16437	3.9	46.2	0	1.77
	e (C_{2v})	-16600.19694	4.0	25.9	0	2.45
	f (C_{2v})	-16600.18298	3.9	34.5	1–> b(D_{2d})	5.59
	g (C_{2h})	-16600.19224	3.9	28.7	0	2.231
	h (C_s)	-16600.16301	3.8	47.0	1	1.623
	i (D_3)	-16600.19224	3.9	28.7	0	2.231
	j (C_{2v})	-16600.20441	4.0	21.2	1–> b(D_{2d})	1.88



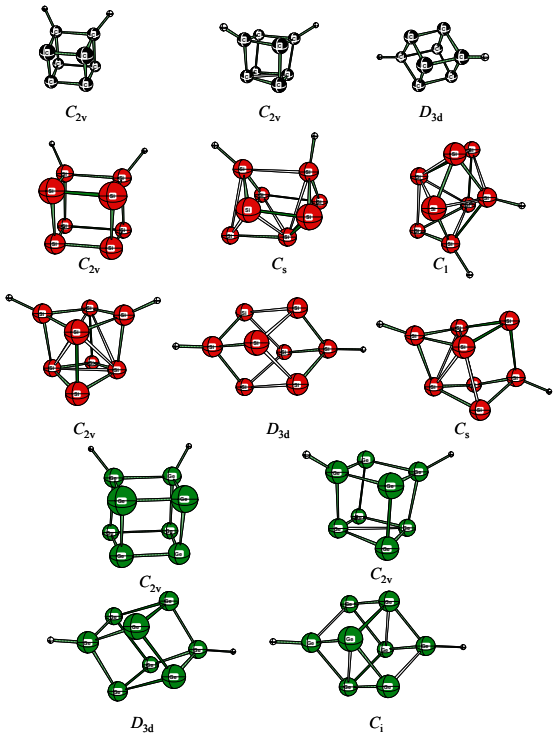
S-Figure 1. B3LYP/6-31G* optimized Si_8^{2-} isomers



S-Figure 2. B3LYP/6-31G* optimized Ge_8^{2-} isomers

S-Table 3. Total energies, relative energies, number of imaginary frequencies, zero-point energies and HOMO-LUMO gap energies of isomers of X_8H_2 (X=C, Si and Ge) (see S-Figure 3)

Species	Symm	E_{tot} (au)	E_{rel} (Kcal/mol)	NIMAG	ZPE (Kcal/mol)	Gap (eV)
1,2- C_8H_2	C_{2v}	-305.52293	6.2	0	37.3	3.62
1,3- C_8H_2	C_{2v}	-305.53289	0.0	0	37.0	3.82
1,4- C_8H_2	D_{3d}	-305.50704	16.2	0	39.3	2.41
1,2- Si_8H_2	C_{2v}	-2317.04872	20.6	2	16.7	2.34
	C_s	-2317.06189	12.3	1	16.6	2.46
	C_1	-2317.07491	4.1	0	17.0	2.62
1,3- Si_8H_2	C_{2v}	-2317.08149	0.0	0	17.3	2.85
1,4- Si_8H_2	D_{3d}	-2317.02982	32.4	3	15.9	1.41
	C_s	-2317.04811	21.0	0	16.8	1.83
1,2- Ge_8H_2	C_{2v}	-16601.38560	9.3	0	13.7	1.88
1,3- Ge_8H_2	C_{2v}	-16601.40044	0.0	0	14.1	2.59
1,4- Ge_8H_2	D_{3d}	-16601.35993	25.4	2	13.8	1.08
	C_i	-16601.38005	12.8	0	14.4	1.65



S-Figure 3. Optimized structurs of 1,3-X_8H_2 (X=C, Si and Ge)