Supporting Information available for

A template for a planar tetracoordinate heavier group 14 atom: Global study of $C_2Si_2X^q$ (X=C, Si, Ge, Sn, Pb; q=+1, 0, -1)

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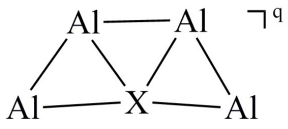
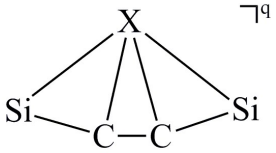
S1. Scheme S1. The pentaatomic planar tetracoordinate X in literatures

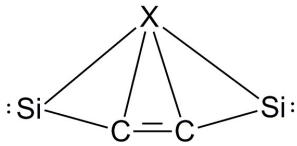


16e q=0 X=Si/Ge
17e q=-1 X=Si/Ge/Sn
18e q=-2 X=Si/Ge



19e q=+1X=Si
20e q=0 X=Si/Ge
21e q=-1 X=Si

S2. Scheme S2. Possible resonant valence structures of global minimum C_2Si_2X



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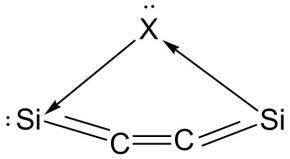

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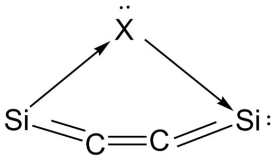


3

Form 1 should be dominant with significant contribution from the forms 2 and 3. The latter two should have equal importance. Note that "→" describes the donor-accepter interaction from the electron lone-pair (Si/X) to the vacant orbital (X/Si).

S3. In consideration of the reliability of the B3LYP functional, we utilized the other

two functionals (M06-2X[1] and PBE0[2]) to assess the computed structural parameters of the key structures. The computed bond distances of the global structure of each system at the three density functional levels are shown in Table S1. The M06-2X and PBE0 predict very close bond distances to each other. For the SiCCSi skeleton, the three functionals produce very similar results. The distance between X and C_2/C_3 is similar at the three functional levels. Yet the X-Si_1/Si_4 distances at B3LYP are somewhat longer than at M06-2x and PBE0. Note that for X=Sn/Pb with q=0, the ptX is asymmetric, and we used the average X-Si_1/Si_4 bond values for comparison.

In addition, for the three low-lying isomers of each system, we calculated the single-point energies at the CCSD(T)/def2-TZVPP//M06-2X/def2-TZVPP and CCSD(T)/def2-TZVPP//PBE0/def2-TZVPP level. The energies were summarized in Table S2. We can find that the relative energies of the three low-lying isomers are very similar at the three single-point levels. Clearly, the three functionals lead to the same conclusion. This is understandable since all the three functionals predict very similar structure of the cumulenic SiCCSi skeleton, which should contribute most to the stabilization of the whole system.

Table S1. The bond lengths(Å) of global minimum $C_2Si_2X^q$(X= Si, Ge, Sn, Pb; q=0,±1) at the B3LYP/def2-TZVPP, M06-2X/def2-TZVPP and PBE0/def2-TZVPP

			X-Si_1	X-C_2	X-C_3	X-Si_4	Si_1-C_2	C_2-C_3	C_3-Si_4
		B3LYP	2.740	1.977	1.977	2.740	1.762	1.322	1.762
	+1	M06-2X	2.673	1.960	1.960	2.673	1.758	1.321	1.758
		PBE0	2.633	1.961	1.961	2.633	1.765	1.321	1.765
		B3LYP	2.602	1.925	1.925	2.602	1.717	1.363	1.717
X=Si	0	M06-2X	2.551	1.913	1.913	2.551	1.710	1.368	1.710
		PBE0	2.527	1.912	1.912	2.527	1.719	1.364	1.719
		B3LYP	2.460	2.065	2.065	2.460	1.751	1.316	1.751
	-1	M06-2X	2.419	2.035	2.035	2.419	1.750	1.316	1.750
		PBE0	2.407	2.033	2.033	2.407	1.755	1.318	1.755
		B3LYP	2.872	2.115	2.115	2.872	1.758	1.318	1.758
	+1	M06-2X	2.790	2.097	2.097	2.790	1.756	1.316	1.756
		PBE0	2.769	2.094	2.094	2.769	1.759	1.318	1.759
		B3LYP	2.737	2.057	2.057	2.737	1.716	1.359	1.716
X=Ge	0	M06-2X	2.671	2.042	2.042	2.671	1.710	1.364	1.710
		PBE0	2.655	2.036	2.036	2.655	1.716	1.361	1.716
		B3LYP	2.612	2.226	2.226	2.612	1.739	1.316	1.739
	-1	M06-2X	2.556	2.187	2.187	2.556	1.737	1.317	1.737
		PBE0	2.534	2.180	2.180	2.534	1.743	1.317	1.743
		B3LYP	3.083	2.343	3.343	3.083	1.754	1.313	1.754
	+1	M06-2X	3.016	2.331	2.331	3.016	1.749	1.311	1.749
		PBE0	2.991	2.317	2.317	2.991	1.753	1.313	1.753
		B3LYP	2.790	2.236	2.335	3.156	1.731	1.345	1.707
X=Sn	0	M06-2X	2.885	2.255	2.255	2.885	1.707	1.359	1.707
		PBE0	2.867	2.245	2.245	2.867	1.713	1.355	1.713
		B3LYP	2.892	2.428	2.428	2.892	1.724	1.320	1.724
	-1	M06-2X	2.842	2.407	2.407	2/842	1.715	1.325	1.715
		PBE0	2.795	2.385	2.385	2.795	1.727	1.321	1.727
		B3LYP	3.180	2.451	2.451	3.180	1.752	1.310	1.752
	+1	M06-2X	3.122	2.436	2.436	3.122	1.744	1.310	1.744
		PBE0	3.096	2.422	2.422	3.096	1.749	1.311	1.749
		B3LYP	2.812	2.343	2.540	3.399	1.741	1.331	1.705

X=Pb	0	M06-2X	2.975	2.358	2.358	2.975	1.706	1.356	1.706
		PBE0	2.967	2.348	2.348	2.967	1.712	1.352	1.712
		B3LYP	3.026	2.536	2.536	3.026	1.719	1.321	1.719
	-1	M06-2X	2.986	2.525	2.525	2.986	1.706	1.328	1.706
		PBE0	2.923	2.492	2.492	2.923	1.720	1.322	1.720

S4. Table S2. The relative energies(in kcal/mol) of global minimum $C_2Si_2X^q$(X= Si, Ge, Sn, Pb; q=0,±1) at CCSD(T)/def2-TZVPP//M06-2X/def2-TZVPP, CCSD(T)/ def2-TZVPP//PBE0/def2-TZVPP and CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP

			CCSD(T)/def2-TZVPP//M06-2X/def2-TZVPP+ZPVE	CCSD(T)/def2-TZVPP//PBE0/def2-TZVPP+ZPVE	CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP+ZPVE C
X=Si	+1	01	0.00	0.00	0.00
		02	31.37	31.36	31.22
	0	01	0.00	0.00	0.00
		02	15.30	15.15	15.01
		03	17.38	17.17	17.21
	-1	01	0.00	0.00	0.00
		02	4.92	4.85	4.84
		03	5.29	5.02	5.39
X=Ge	+1	01	0.00	0.00	0.00
		02	1.97	2.06	1.69
		03	12.16	12.46	11.54
	0	01	0.00	0.00	0.00
		02	1.57	1.84	1.46
		03	12.19	12.19	12.01
	-1	01	0.00	0.00	0.00
		02	3.95	4.13	3.76
		03	4.28	4.23	4.36
X=Sn	+1	01	0.00	0.00	0.00
		02	5.01	3.96	4.02
		03	14.07	14.52	13.11
	0	01	0.00	0.00	0.00
		02	6.87	7.13	5.84
		03	14.17	14.12	13.11
	-1	01	0.00	0.00	0.00
		02	6.73	6.55	6.45
		03	6.73	6.55	6.96
X=Pb	+1	01	0.00	0.00	0.00
		02	6.86	5.66	5.63
		03	7.30	5.66	7.09
	0	01	0.00	0.00	0.00
		02	9.34	9.41	7.17
		03	13.10	12.96	11.06
	-1	01	0.00	0.00	0.00
		02	6.28	6.25	6.03
		03	13.32	13.59	13.86

S5. In addition to the low spin state, we also studied the higher spin state of $C_2Si_2X^q$ (X=C, Si, Ge, Sn, Pb), i.e., triplet for q=0 and quartet for q=+1, -1. As shown in Table S3, the energy gap between the low and high spin states shows that in general, low spin state structures are energetically more stable than the high spin state.

Table S3. The T1 diagnostic and the energy gap between the low and high spin states (ΔE_{S-T}) of global minimum $C_2Si_2X^q$(X= C, Si, Ge, Sn, Pb; q=0,±1) at the level of CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP

	q	ΔE	T1 diagnostic
X=C	+1	38.92	0.036
	0	38.27	0.023
	-1	34.87	0.053
X=Si	+1	58.31	0.018
	0	18.96	0.017
	-1	33.22	0.021
X=Ge	+1	47.22	0.016
	0	15.26	0.015
	-1	32.99	0.018
X=Sn	+1	43.07	0.016
	0	13.73	0.016
	-1	34.25	0.017
X=Pb	+1	41.96	0.016
	0	11.63	0.017
	-1	33.71	0.017

S6. Table S4. The Mayer Bond Orders of global minimum $C_3Si_2^q$(q=0,±1) at the level of B3LYP/def2-TZVPP

	Si_1-C_2	C_2-C_3	C_3-C_4	C_4-Si_5
$C_3Si_2^+$	1.228	1.945	1.945	1.228
C_3Si_2	1.490	2.050	2.050	1.490
$C_3Si_2^-$	1.425	2.167	2.167	1.425

S7. Table S5. The Mayer Bond Orders of global minimum $C_2Si_2X^q$(X= Si, Ge, Sn, Pb; q=0,±1) at the level of B3LYP/def2-TZVPP

	q	X-Si_1	X-C_2	X-C_3	X-Si_4	Si_1-C_2	C_2-C_3	C_3-Si_4
	+1	0.409	0.724	0.724	0.409	1.162	1.473	1.162
X=Si	0	0.541	0.778	0.778	0.541	1.487	1.242	1.487
	-1	0.869	0.459	0.459	0.869	1.431	1.555	1.431
	+1	0.387	0.654	0.654	0.387	1.200.	1.533	1.200
X=Ge	0	0.480	0.731	0.731	0.480	1.515	1.303	1.515
	-1	0.697	0.415	0.415	0.697	1.518	1.606	1.518
	+1	0.392	0.549	0.549	0.392	1.238	1.663	1.238
X=Sn	0	0.653	0.702	0.454	0.385	1.478	1.495	1.605
	-1	0.590	0.314	0.314	0.590	1.622	1.697	1.622
	+1	0.386	0.516	0.516	0.386	1.248	1.665	1.248
X=Pb	0	0.744	0.692	0.383	0.374	1.412	1.573	1.605
	-1	0.517	0.317	0.317	0.517	1.648	1.697	1.648

S8. Table S6. The natural charge of global minimum $C_2Si_2X^q$(X= Si, Ge, Sn, Pb; q=0,±1) at the level of B3LYP/def2-TZVPP

	q	X	Si_1	C_2	C_3	Si_4
X=Si	+1	0.865	1.033	-0.966	-0.966	1.033
	0	0.807	0.633	-1.037	-1.037	0.633
	-1	0.264	0.215	-0.847	-0.847	0.215
X=Ge	+1	0.904	1.017	-0.969	-0.969	1.017
	0	0.828	0.626	-1.040	-1.040	0.626
	-1	0.201	0.247	-0.848	-0.848	0.247
X=Sn	+1	1.047	0.937	-0.961	-0.961	0.937
	0	0.888	0.494	-0.962	-1.063	0.643
	-1	0.239	0.268	-0.888	-0.888	0.268
X=Pb	+1	1.075	0.906	-0.944	-0.944	0.906
	0	0.836	0.447	-0.901	-1.021	0.639
	-1	0.222	0.276	-0.887	-0.887	0.276

S9. Table S7. The spin density of global minimum $C_2Si_2X^q$(X= Si, Ge, Sn, Pb; q=0,±1) at the level of B3LYP/def2-TZVPP

	q	Si_1	C_2	C_3	Si_4	Si_5
	+1	0.318	0.190	0.190	0.318	-0.015
X=Si	-1	0.060	0.077	0.077	0.060	0.727
	+1	0.324	0.186	0.186	0.324	-0.021
X=Ge	-1	0.030	0.060	0.060	0.030	0.820
	+1	0.333	0.179	0.179	0.333	-0.025
X=Sn	-1	-0.003	0.038	0.038	-0.003	0.930
	+1	0.340	0.175	0.175	0.340	-0.029
X=Pb	-1	-0.013	0.028	0.028	-0.013	0.970

S10. It's of interest to find in Table S8 that both the VDE and ADE of $C_2Si_2X^-$ indicate the mono-anionic $C_2Si_2X^-$ is stable with respect to the auto electron-detachment. So $C_2Si_2X^-$ may be observed in the photo-electron spectroscopic experiments.

Table S8. The vertical detachment energies (VDE), the adiabatic detachment energy (ADE), the vertical ionization potential (VIP) and the adiabatic ionization potential (AIP) of global minimum $C_2Si_2X^q$ (X= Si, Ge, Sn, Pb; q=0,±1) at the level of CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP

	ADE	VDE	AIP	VIP
X=Si	32.16	39.18	171.70	174.59
X=Ge	35.03	42.27	168.29	169.99
X=Sn	38.44	42.86	161.17	163.57
X=Pb	38.90	42.18	155.52	158.84

S11. Table S9. For the obtained isomers within 30kcal/mol, the energies(in a.u.), zero-point energies(in a.u.) and the relative energies(in kcal/mol) at B3LYP/def2-TZVPP and CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP

$C_3Si_2^+$	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-692.937106	0.013836	-692.923270	0.00	-691.733202	-691.719366	0.0(	0.0
02	-692.887232	0.012914	-692.874318	30.72	-691.702664	-691.689750	18.5	0.0

C_3Si_2	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-693.235431	0.015365	-693.220066	0.00	-692.033584	-692.018219	0.0(	0.0
02	-693.165580	0.013225	-693.152355	42.49	-691.984115	-691.970890	29.7(	0.0

$C_3Si_2^-$	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-693.2958200	0.014184	-693.281636	0.00	-692.089864	-692.075680	0.0(	0.0
02	-693.2540510	0.013605	-693.240446	25.85	-692.056164	-692.042559	20.7	0.0
03	-693.2532520	0.013486	-693.239766	26.27	-692.056011	-692.042525	20.8	0.0
04	-693.2124196	0.011263	-693.201157	50.50	-692.030462	-692.030462	35.4	0.0

$C_2Si_3^+$	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-944.385631	0.011181	-944.374450	0.00	-942.818226	-942.807045	0.0(	0.0
02	-944.342367	0.010483	-944.331884	26.71	-942.767773	-942.757290	31.2	0.0

C_2Si_3	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-944.652965	0.011796	-944.641169	0.00	-943.092465	-943.080669	0.0(	0.0
02	-944.614841	0.010899	-944.603942	23.36	-943.067643	-943.056744	15.0	0.0
03	-944.623250	0.011139	-944.612111	18.23	-943.064388	-943.053249	17.2	0.0
04	-944.610883	0.010731	-944.600152	25.74	-943.051891	-943.041160	24.7	0.0

$C_2Si_3^-$	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-944.705244	0.011496	-944.693748	0.00	-943.143571	-943.132075	0.00	0.0
02	-944.687804	0.009986	-944.677818	10.00	-943.134348	-943.124362	4.84	0.0
03	-944.68999	0.010484	-944.679506	8.94	-943.133977	-943.123493	5.39	0.0
04	-944.702626	0.011110	-944.691516	1.40	-943.128774	-943.117664	9.04	0.0
05	-944.671363	0.010201	-944.661162	20.45	-943.122053	-943.111852	12.69	0.0
06	-944.679575	0.010466	-944.669109	15.46	-943.119658	-943.109192	14.36	0.0
07	-944.680464	0.009992	-944.670472	14.61	-943.115992	-943.106000	16.36	0.0
08	-944.679161	0.010665	-944.668496	15.85	-943.116289	-943.105624	16.60	0.0
09	-944.677014	0.010032	-944.666982	16.80	-943.110113	-943.100081	20.08	0.0
10	-944.667512	0.010305	-944.657207	22.93	-943.105495	-943.095190	23.15	0.0
11	-944.663288	0.009165	-944.654123	24.87	-943.103291	-943.094126	23.81	0.0
12	-944.666514	0.009920	-944.656594	23.31	-943.101611	-943.091691	25.34	0.0

$C_2Si_2Ge^+$	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-2731.944929	0.010716	-2731.934213	0.00	-2729.394206	-2729.38349	0.0(	0.0
02	-2731.941384	0.010569	-2731.930815	2.13	-2729.391365	-2729.38080	1.6	0.0

03	-2731.922494	0.009789	-2731.912705	13.50	-2729.374886	-2729.36510	11.5	0.0
04	-2731.922431	0.009903	-2731.912528	13.61	-2729.374376	-2729.36447	11.9	0.0

C_2Si_2Ge	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-2732.204669	0.011052	-2732.193617	0.00	-2729.662736	-2729.65168	0.0	0.0
02	-2732.201963	0.011040	-2732.190923	1.69	-2729.660398	-2729.64936	1.4	0.0
03	-2732.184190	0.010662	-2732.173528	12.61	-2729.643213	-2729.63255	12.0	0.0
04	-2732.179407	0.010510	-2732.168897	15.51	-2729.638824	-2729.62831	14.6	0.0
05	-2732.175387	0.010387	-2732.165000	17.96	-2729.635433	-2729.62505	16.7	0.0
06	-2732.166500	0.010442	-2732.156058	23.57	-2729.626332	-2729.61589	22.4	0.0
07	-2732.165398	0.010354	-2732.155044	24.20	-2729.624523	-2729.61417	23.5	0.0
08	-2732.161803	0.009715	-2732.152088	26.06	-2729.621112	-2729.61140	25.2	0.0
09	-2732.160964	0.009841	-2732.151123	26.67	-2729.619553	-2729.60971	26.3	0.0

$C_2Si_2Ge^-$	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-2732.260874	0.010950	-2732.249924	0.00	-2729.718455	-2729.70751	0.00	0.0
02	-2732.254159	0.010757	-2732.243402	4.09	-2729.712266	-2729.70151	3.76	0.0
03	-2732.248356	0.010008	-2732.238348	7.26	-2729.710561	-2729.70055	4.36	0.0
04	-2732.246496	0.009914	-2732.236582	8.37	-2729.709103	-2729.69919	5.22	0.0
05	-2732.237831	0.009254	-2732.228577	13.40	-2729.704166	-2729.69491	7.90	0.0
06	-2732.240576	0.009700	-2732.230876	11.95	-2729.703936	-2729.69424	8.33	0.0
07	-2732.260835	0.010730	-2732.250105	-0.11	-2729.704299	-2729.69357	8.74	0.0
08	-2732.241483	0.010038	-2732.231445	11.60	-2729.699358	-2729.68932	11.41	0.0
09	-2732.251536	0.010386	-2732.241150	5.51	-2729.697666	-2729.68728	12.69	0.0
10	-2732.241538	0.010243	-2732.231295	11.69	-2729.697355	-2729.68711	12.80	0.0

11	-2732.241081	0.009515	-2732.231566	11.52	-2729.694812	-2729.68530	13.94	0.02
12	-2732.234802	0.010056	-2732.224746	15.80	-2729.690901	-2729.68085	16.73	0.04
13	-2732.229519	0.009699	-2732.219820	18.89	-2729.690230	-2729.68053	16.93	0.03
14	-2732.234324	0.009426	-2732.224898	15.70	-2729.689283	-2729.67986	17.35	0.03
15	-2732.237946	0.009967	-2732.227979	13.77	-2729.688734	-2729.67877	18.03	0.02
16	-2732.230806	0.009945	-2732.220861	18.24	-2729.687556	-2729.67761	18.76	0.04
17	-2732.223741	0.008931	-2732.214810	22.03	-2729.681511	-2729.67258	21.92	0.02
18	-2732.224653	0.009220	-2732.215433	21.64	-2729.681061	-2729.67184	22.38	0.05
19	-2732.224142	0.009903	-2732.214239	22.39	-2729.678799	-2729.66890	24.23	0.02
20	-2732.219414	0.009686	-2732.209728	25.22	-2729.675724	-2729.66604	26.02	0.03
21	-2732.219695	0.009712	-2732.209983	25.06	-2729.674536	-2729.66482	26.78	0.04
22	-2732.234884	0.010420	-2732.224464	15.98	-2729.673291	-2729.66287	28.01	0.04
23	-2732.215496	0.009399	-2732.206097	27.50	-2729.670795	-2729.66140	28.93	0.04

$C_2Si_2Sn^+$	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-869.299621	0.010538	-869.289083	0.00	-867.478262	-867.467724	0.00	0.01
02	-869.291278	0.010199	-869.281079	5.02	-867.471508	-867.461309	4.02	0.02
03	-869.27218	0.009503	-869.262677	16.57	-867.456329	-867.446826	13.11	0.02

C_2Si_2Sn	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-869.549202	0.010899	-869.538303	0.00	-867.735458	-867.724559	0.00	0.01
02	-869.536396	0.010508	-869.525888	7.79	-867.725763	-867.715255	5.84	0.01
03	-869.526196	0.010366	-869.515830	14.10	-867.714025	-867.703659	13.11	0.02
04	-869.524141	0.010185	-869.513956	15.28	-867.713337	-867.703152	13.43	0.02
05	-869.513009	0.009865	-869.503144	22.06	-867.702987	-867.693122	19.73	0.02

06	-869.512084	0.010134	-869.501950	22.81	-867.701157	-867.691023	21.0	0.0
07	-869.504959	0.009757	-869.495202	27.05	-867.699110	-867.689353	22.0	0.0
08	-869.511139	0.010026	-869.501113	23.34	-867.698776	-867.688750	22.4	0.0
09	-869.507527	0.009563	-869.497964	25.31	-867.698140	-867.688577	22.5	0.0
10	-869.507205	0.010161	-869.497044	25.89	-867.695714	-867.685553	24.4	0.0

$C_2Si_2Sn^-$	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-869.610650	0.010902	-869.599748	0.0	-867.796722	-867.785820	0.0	0.0
02	-869.591868	0.009466	-869.582402	10.8	-867.785007	-867.775541	6.4	0.0
03	-869.592291	0.009622	-869.582669	10.7	-867.784355	-867.774733	6.9	0.0
04	-869.591391	0.009640	-869.581751	11.2	-867.782649	-867.773009	8.0	0.0
05	-869.591426	0.010006	-869.581420	11.5	-867.779123	-867.769117	10.4	0.0
06	-869.603574	0.010461	-869.593113	4.1	-867.775798	-867.765337	12.8	0.0
07	-869.590020	0.010020	-869.580000	12.3	-867.772711	-867.762691	14.5	0.0
08	-869.584735	0.009798	-869.574937	15.5	-867.771167	-867.761369	15.3	0.0
09	-869.577944	0.009193	-869.568751	19.4	-867.770369	-867.761176	15.4	0.0
10	-869.577287	0.009601	-869.567686	20.1	-867.770603	-867.761002	15.5	0.0
11	-869.586027	0.010009	-869.576018	14.8	-867.770070	-867.760061	16.1	0.0
12	-869.579873	0.009588	-869.570285	18.4	-867.766638	-867.757050	18.0	0.0
13	-869.580885	0.009852	-869.571033	18.0	-867.766115	-867.756263	18.5	0.0
14	-869.580898	0.009148	-869.571750	17.5	-867.763911	-867.754763	19.4	0.0
15	-869.581745	0.009786	-869.571959	17.4	-867.761466	-867.751680	21.4	0.0
16	-869.569970	0.009340	-869.560630	24.5	-867.759583	-867.750243	22.3	0.0
17	-869.575123	0.009739	-869.565384	21.5	-867.759260	-867.749521	22.7	0.0
18	-869.569221	0.009496	-869.559725	25.1	-867.754852	-867.745356	25.3	0.0
19	-869.567438	0.008708	-869.558730	25.7	-867.753734	-867.745026	25.6	0.0
20	-869.584255	0.010224	-869.574031	16.1	-867.751531	-867.741307	27.9	0.0

$C_2Si_2Pb^+$	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-847.875022	0.01049	-847.864532	0.0	-846.110695	-846.100205	0.0(	0.0
02	-847.863661	0.009963	-847.853698	6.8	-846.101191	-846.091228	5.6	0.0
03	-847.863826	0.010053	-847.853773	6.7	-846.098964	-846.088911	7.0	0.0
04	-847.846036	0.009457	-847.836579	17.5	-846.088044	-846.078587	13.5(	0.0
05	-847.846826	0.009773	-847.837053	17.2	-846.087124	-846.077351	14.3	0.0

C_2Si_2Pb	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-848.118019	0.010837	-848.107182	0.0	-846.358887	-846.348050	0.0(	0.0
02	-848.100365	0.010226	-848.090139	10.6	-846.346853	-846.336627	7.1	0.0
03	-848.096251	0.010223	-848.086028	13.2	-846.340642	-846.330419	11.0(	0.0
04	-848.093406	0.009972	-848.083434	14.9	-846.339658	-846.329686	11.5	0.0
05	-848.083946	0.009987	-848.073959	20.8	-846.329321	-846.319334	18.0	0.0
06	-848.080011	0.009553	-848.070458	23.0	-846.327338	-846.317785	18.9	0.0
07	-848.075398	0.009598	-848.065800	25.9	-846.326322	-846.316724	19.6(	0.0
08	-848.079038	0.009568	-848.069470	23.6	-846.325963	-846.316395	19.8(	0.0
09	-848.078896	0.009950	-848.068946	23.9	-846.323016	-846.313066	21.9	0.0
10	-848.076061	0.009968	-848.066093	25.7	-846.321223	-846.311255	23.0	0.0

$C_2Si_2Pb^-$	B3LYP/def2-TZVPP				CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP			
	E	ZPVE	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	T1
01	-848.179482	0.010793	-848.168689	0.0	-846.420837	-846.410044	0.0(	0.0
02	-848.160825	0.009395	-848.151430	10.8	-846.409823	-846.400428	6.0	0.0
03	-848.171454	0.010377	-848.161077	4.7	-846.398335	-846.387958	13.8(	0.0

04	-848.154434	0.009766	-848.144668	15.0	-846.397019	-846.387253	14.3(	0.0
05	-848.147535	0.009674	-848.137861	19.3	-846.396009	-846.386335	14.8	0.0
06	-848.153229	0.009657	-848.143572	15.7	-846.394808	-846.385151	15.6	0.0
07	-848.154780	0.009880	-848.144900	14.9	-846.394394	-846.384514	16.0	0.0
08	-848.154260	0.009662	-848.144598	15.1	-846.393579	-846.383917	16.3	0.0
09	-848.154863	0.009798	-848.145065	14.8	-846.393370	-846.383572	16.6	0.0
10	-848.142039	0.008843	-848.133196	22.2	-846.390400	-846.381557	17.8	0.0
11	-848.147402	0.009636	-848.137766	19.4	-846.388330	-846.378694	19.6	0.0
12	-848.148186	0.008946	-848.139240	18.4	-846.386679	-846.377733	20.2	0.0
13	-848.146489	0.009598	-848.136891	19.9	-846.385712	-846.376114	21.2	0.0
14	-848.150374	0.009655	-848.140719	17.5	-846.385226	-846.375571	21.6	0.0
15	-848.146634	0.009430	-848.137204	19.7	-846.384596	-846.375166	21.8	0.0
16	-848.135756	0.008610	-848.127146	26.0	-846.376875	-846.368265	26.2	0.0
17	-848.155104	0.010068	-848.145036	14.8	-846.377375	-846.367307	26.8	0.0

S12. Table S10. Optimized geometries (in angstrom) of the isomers in Table S9 at the level of B3LYP/def2-TZVPP.

$C_3Si_2^+$	Cartesian Coordinates			
01	6	1.281611	0.000005	0.000152
	6	-0.000102		-0.000326
	6	-1.281839	0.000894	0.000326
	14	3.021118	0.000002	-0.000052
	14	-3.021337	-0.000108	-0.000053
02	6	0.680750	-0.902149	0.000000
	6	0.000571	0.393034	0.000000
	6	-0.690739	-0.895814	0.000000
	14	-2.046583	0.310404	0.000000
	14	2.050438	0.286955	0.000000

C_3Si_2	Cartesian Coordinates			
01	6	0.000000	0.000000	-1.285737
	6	0.000000	0.000000	-0.000024
	6	0.000000	0.000000	1.285693
	14	0.000000	0.000000	-2.970989
	14	0.000000	0.000000	2.970941
02	14	2.013499	0.284773	0.000000
	6	0.707718	-0.874276	0.000000
	6	0.000038	0.395612	0.000000
	6	-0.710221	-0.872364	0.000000
	14	-2.012384	0.291243	0.000000

$C_3Si_2^-$	Cartesian Coordinates			
01	6	-1.292646	0.000302	0.000016
	14	-2.995519	0.000868	0.000480
	6	-0.000108	0.000282	0.000081
	14	2.995281	0.001898	0.000026
	6	1.292536	0.000599	0.000041
02	14	1.626050	-0.255142	0.000000
	6	0.000000	0.456551	0.000000
	14	-0.336634	-1.437539	0.000000
	6	-1.022415	1.334051	0.000000
	6	-1.986222	2.158988	0.000000
03	6	0.586353	1.855176	0.000000
	6	0.000000	0.653274	0.000000
	14	2.016615	0.759333	0.000000
	6	-0.832780	-0.385019	0.000000
	14	-1.911003	-1.669375	0.000000
04	14	-1.793166	0.378317	0.000000
	6	-0.632264	-1.182940	0.000000
	6	0.000039	0.564278	0.000000
	14	1.793149	0.376778	0.000000

	6	0.631177	-1.183397	0.000000

$C_2Si_3^+$	Cartesian Coordinates			
01	14	-0.000014	0.000000	-0.000040
	6	-0.000069	0.000000	1.976987
	6	1.245579	0.000000	1.535255
	14	-1.756456	0.000000	2.102352
	14	2.688545	0.000000	0.526068
02	14	1.247615	1.577775	0.000000
	14	-0.980320	1.764147	0.000000
	6	0.000000	0.121785	0.000000
	14	-0.226897	-2.900583	0.000000
	6	-0.094262	-1.151576	0.000000

C_2Si_3	Cartesian Coordinates			
01	14	0.000000	0.000000	0.000000
	6	0.000000	0.000000	1.925000
	6	1.274914	0.000000	1.442296
	14	-1.716983	0.000000	1.955089
	14	2.581283	0.000000	0.327694
02	6	0.000000	1.025090	-0.000098
	14	0.000000	0.000000	1.580046
	14	-1.368451	0.000000	-0.789981
	6	0.000000	-1.025090	-0.000098
	14	1.368451	0.000000	-0.789981
03	6	-1.035278	-1.023889	0.910323
	6	0.168407	-0.888097	0.419827
	14	-1.610888	-0.010402	-0.556581
	14	1.739788	-0.406285	-0.347132
	14	0.242617	1.236109	0.333649
04	14	2.064030	0.000264	-0.000098
	6	0.383388	-0.538696	0.507956
	6	0.383067	0.538541	-0.507507
	14	-1.196537	1.210846	0.096739
	14	-1.195973	-1.211044	-0.096834

$C_2Si_3^-$	Cartesian Coordinates			
01	14	-2.193457	-0.101800	0.000000
	6	-0.657801	-0.944305	0.000000
	14	0.000000	1.012938	0.000000
	6	0.657810	-0.944282	0.000000
	14	2.193453	-0.101744	0.000000
02	6	-1.579083	0.587572	0.000000
	6	-0.322462	1.006727	0.000000
	14	-0.322462	-0.596009	1.267238
	14	1.459873	0.508746	0.000000

	14	-0.322462	-0.596009	-1.267238
03	6	-1.164065	-0.195252	1.277795
	14	0.184881	1.356680	-0.094351
	6	0.080962	-0.468562	0.960496
	14	1.512945	-0.602446	-0.162167
	14	-1.233639	-0.469742	-0.702749
04	14	-1.227654	1.736623	0.000000
	6	0.000000	0.410285	0.000000
	14	-1.735473	-0.474910	0.000000
	6	1.083160	-0.335245	0.000000
	14	2.498915	-1.293873	0.000000
05	14	1.511276	-0.664904	0.000000
	6	0.000124	-0.182326	0.984753
	6	0.000124	-0.182326	-0.984753
	14	-1.511506	-0.663818	0.000000
	14	0.000124	1.485002	0.000000
06	6	-2.330127	-0.188462	0.310631
	14	-0.469937	-1.089842	-0.246562
	6	-1.365346	0.625852	0.157092
	14	1.727762	-0.448189	0.193484
	14	0.325949	1.350579	-0.147375
07	14	-1.900388	-0.000391	0.137480
	14	0.032025	-1.218573	-0.118033
	14	0.031409	1.218811	-0.117934
	6	1.515606	0.000787	0.007660
	6	2.770621	-0.000430	0.222142
08	6	-1.730557	-0.901752	0.623631
	14	-1.241079	0.663506	-0.454342
	6	-0.501181	-1.115996	0.324097
	14	0.961976	1.219694	0.333554
	14	1.235563	-1.018451	-0.285381
09	14	1.148243	-1.460212	0.000000
	14	0.000000	0.485372	0.000000
	14	-1.142275	-1.464697	0.000000
	6	-0.004612	2.217020	0.000000
	6	-0.009313	3.475233	0.000000
10	14	2.102172	-0.345237	-0.070241
	6	0.828548	0.810459	0.313253
	6	0.131347	-0.431000	-0.016587
	14	-0.956397	1.242717	-0.085304
	14	-1.557158	-1.060106	0.028402
11	6	-2.407670	-0.000288	-0.632997
	6	-2.407956	0.000860	0.633074
	14	-0.615976	-0.000672	-0.000124
	14	1.340080	-1.144272	0.000214
	14	1.339735	1.144699	-0.000122
12	14	1.772172	-0.742957	0.000000
	6	0.061086	-1.192145	0.000000
	6	0.000000	0.299712	0.000000
	14	-1.683520	-0.874229	0.000000

	14	-0.114831	1.999657	0.000000

$C_2Si_2Ge^+$	Cartesian Coordinates			
01	32	0.000000	0.000000	0.000000
	6	0.000000	0.000000	2.115000
	6	1.252405	0.000000	1.704320
	14	-1.750351	0.000000	2.276984
	14	2.758801	0.000000	0.798374
02	6	0.017007	0.630308	0.000000
	14	0.617718	-1.262168	0.000000
	6	1.333546	0.571074	0.000000
	14	2.997453	-0.020680	0.000000
	32	-1.818363	0.263909	0.000000
03	14	-1.728155	1.376844	0.000000
	6	0.021945	1.751161	0.000000
	6	0.001275	0.320658	0.000000
	14	1.760324	1.323711	0.000000
	32	-0.018738	-1.567506	0.000000
04	14	2.426310	-0.722152	-0.006465
	6	0.383080	-0.125381	0.041021
	6	1.462384	0.769648	-0.062532
	14	-0.057842	1.791677	-0.061349
	32	-1.411025	-0.728625	0.149446

C_2Si_2Ge	Cartesian Coordinates			
01	32	0.000000	0.000000	0.000000
	6	0.000000	0.000000	2.057000
	6	1.282899	0.000000	1.607924
	14	-1.714270	0.000000	2.133647
	14	2.670719	0.000000	0.598690
02	6	1.360211	0.593617	0.000000
	14	2.912957	-0.159426	0.000000
	6	0.008821	0.721975	0.000000
	32	-1.760019	0.305402	0.000000
	14	0.540173	-1.142090	0.000000
03	6	1.337627	1.022727	0.999668
	32	-0.400733	-0.958016	0.120284
	6	0.148719	1.194667	0.488205
	14	-1.463487	1.156961	-0.340057
	14	1.753278	0.097704	-0.565519
04	6	-0.419925	-1.125223	1.130533
	14	0.729678	1.220708	0.450719
	6	0.685503	-0.919065	0.475405
	14	2.116107	-0.372155	-0.510085
	32	-1.294827	0.012062	-0.275141
05	6	1.491556	-1.034869	0.935067
	6	0.268835	-0.815387	0.553684
	14	2.035907	-0.154762	-0.636271

	14	0.422329	1.314438	0.345418
	32	-1.405552	-0.160435	-0.151893
	6	1.886163	2.114512	0.000000
	6	1.843196	0.837722	0.000000
06	14	0.000000	1.306443	0.000000
	14	1.164907	-0.867219	0.000000
	32	-1.208901	-0.745704	0.000000
	14	2.356102	-0.473673	-0.040330
	6	0.662043	-0.281973	0.619315
07	6	0.957367	0.679310	-0.427156
	14	-0.426454	1.754283	0.064219
	32	-1.147861	-0.634767	-0.046481
	32	-1.549406	0.000266	-0.005959
	6	0.226968	0.000117	0.280308
08	14	1.347253	1.568985	-0.170472
	14	1.346053	-1.569481	-0.170468
	6	1.752153	-0.000378	0.547002
	14	1.714621	-1.504479	-0.033679
	6	0.715715	-0.182741	0.344905
09	32	-1.386540	-0.217461	-0.083139
	14	1.222231	1.653134	-0.213772
	6	-0.173490	0.995669	0.675888

$C_2Si_2Ge^-$	Cartesian Coordinates			
	32	0.000000	0.000000	0.000000
	6	0.000000	0.000000	2.226000
01	6	1.256815	0.000000	1.837251
	14	-1.719330	0.000000	1.966328
	14	2.529269	0.000000	0.652183
	6	0.006976	0.963599	0.000000
	14	0.514694	-1.059836	0.000000
02	6	1.309814	0.831355	0.000000
	14	2.777454	-0.143649	0.000000
	32	-1.684020	0.187929	0.000000
	6	1.287702	-0.660714	1.260592
	6	0.811412	0.510606	0.911175
03	14	1.350717	-0.680630	-0.732740
	14	0.072596	1.752193	-0.204265
	32	-1.011192	-0.440393	0.010368
	6	-0.364477	0.617386	1.604650
	6	0.641979	-0.066075	1.133737
04	32	-1.130658	-0.252806	-0.230117
	14	1.663118	-0.917267	-0.137557
	14	0.807144	1.250252	-0.505119
	6	-1.025442	1.759822	0.000000
	6	0.152267	1.164994	0.000000
05	14	-1.025786	0.047340	1.276157
	32	1.059374	-0.586633	0.000000
	14	-1.025786	0.047340	-1.276157

	6	1.606227	-0.371577	1.254817
	14	1.496595	-0.702883	-0.721380
06	6	0.317248	-0.336770	1.047232
	32	-1.267354	-0.181014	-0.062949
	14	0.587741	1.417074	-0.124493
	14	-1.800124	0.921482	0.000000
	6	-0.004570	0.766734	0.000000
07	32	-0.747778	-1.175015	0.000000
	6	1.301189	0.873348	0.000000
	14	3.002600	1.064048	0.000000
	6	2.729749	-0.448788	-0.382392
	6	1.892564	0.492457	-0.198653
08	14	0.823053	-1.091506	0.295618
	14	0.345488	1.457475	0.172770
	32	-1.371357	-0.168163	-0.095667
	14	2.030375	-1.953787	0.000000
	6	0.745565	-0.671570	0.000000
09	14	-0.193761	-2.386952	0.000000
	6	0.013181	0.410279	0.000000
	32	-0.967089	1.929902	0.000000
	6	2.285927	-0.155037	0.721093
	14	1.103029	-1.117973	-0.495825
10	32	-1.180497	-0.359444	0.144814
	14	0.010506	1.691034	-0.306276
	6	1.424063	0.734836	0.378062
	32	1.467644	-0.000040	0.086485
	14	-0.548940	-1.227179	-0.175579
11	14	-0.548846	1.227264	-0.175545
	6	-2.014068	0.000157	0.030402
	6	-3.251863	-0.000144	0.327635
	6	-0.897295	1.608052	0.811933
	32	-1.098754	-0.249063	-0.231647
12	6	0.269431	1.359164	0.350824
	14	1.793023	0.657374	-0.423089
	14	0.987500	-1.359750	0.454243
	6	-2.455191	-0.509981	0.297310
	6	-1.247013	-0.891186	0.207773
13	14	-1.159004	1.024194	-0.273759
	32	0.737880	-0.848408	-0.062534
	14	1.059080	1.515523	0.200229
	6	2.735063	0.351793	0.311320
	32	0.071966	-0.978931	-0.074652
14	6	1.516020	0.579017	0.038690
	14	-1.932781	0.281492	0.200445
	14	-0.053605	1.557146	-0.179816
	14	1.808454	-0.270274	0.000000
	14	0.000000	0.986350	0.000000
15	32	-0.285316	-1.410263	0.000000
	6	-0.999569	2.402419	0.000000
	6	-1.698473	3.448139	0.000000

16	6	-1.645371	-1.470192	0.623211
	6	-0.422500	-1.156174	0.417546
	14	-1.798726	0.122105	-0.514895
	32	1.240410	-0.275474	-0.126071
	14	-0.150267	1.633136	0.357018
17	6	2.733983	-0.426301	0.633156
	6	2.733603	-0.426336	-0.632970
	14	1.049117	0.193359	-0.000208
	32	-1.217577	-0.648046	0.000028
	14	-0.609335	1.653304	0.000065
18	32	-1.434459	-0.181365	-0.125573
	6	0.383522	-0.804357	0.307634
	14	0.320252	1.358094	0.333872
	6	1.500725	-1.401859	0.663321
	14	2.150976	0.001977	-0.462971
19	6	2.096448	2.411328	0.000000
	6	1.573065	1.227922	0.000000
	14	0.137795	2.598576	0.000000
	14	0.000000	0.222649	0.000000
	32	-0.748319	-1.916645	0.000000
20	32	-1.377045	-0.496343	0.017023
	6	0.602911	-0.283313	-0.087142
	14	-0.216198	1.582943	-0.075998
	14	2.476139	-0.661407	-0.049220
	6	1.468131	0.780223	0.288529
21	14	2.464150	-0.574221	-0.029891
	6	0.649700	-0.404269	-0.321199
	6	1.194193	0.670355	0.452369
	32	-1.312448	-0.538250	0.031070
	14	-0.254509	1.690470	-0.097342
22	14	0.000000	0.000000	-4.406538
	6	0.000000	0.000000	-2.663727
	6	0.000000	0.000000	-1.396073
	14	0.000000	0.000000	0.347051
	32	0.000000	0.000000	2.537238
23	14	2.035513	1.258107	0.000000
	6	1.090602	-0.206724	0.000000
	6	0.000000	0.780706	0.000000
	14	-1.494583	1.602826	0.000000
	32	-0.441144	-1.359280	0.000000

$C_2Si_2Sn^+$	Cartesian Coordinates			
01	50	0.000000	0.000000	0.000000
	6	0.000000	0.000000	2.343000
	6	1.260582	0.000000	1.974989
	14	-1.742060	0.000000	2.543643
	14	2.836969	0.000000	1.206853
02	14	0.239398	3.493094	0.000000
	6	-0.351514	1.821752	0.000000

	14	1.503437	1.204552	0.000000
	6	-0.360868	0.506303	0.000000
	50	-0.038765	-1.556248	0.000000
	6	0.083206	2.212013	0.000000
	14	-1.675501	1.883396	0.000000
03	6	0.000000	0.787536	0.000000
	50	-0.041817	-1.351461	0.000000
	14	1.789188	1.657728	0.000000

C_2Si_2Sn	Cartesian Coordinates			
	50	0.050638	0.000000	0.165965
	6	0.035623	0.000000	2.435338
01	6	1.329977	0.000000	2.040417
	14	-1.676501	0.000000	2.549899
	14	2.814431	0.000000	1.179669
	14	2.828137	1.892289	0.000000
	6	1.127228	1.533775	0.000000
02	14	1.594589	-0.321174	0.000000
	6	-0.005246	0.799595	0.000000
	50	-1.323248	-0.742923	0.000000
	6	1.942508	-0.064265	1.027297
	6	1.201136	0.879026	0.502633
03	14	1.709285	-1.009159	-0.542303
	14	0.084612	2.036480	-0.318883
	50	-0.862619	-0.380288	0.064353
	6	-0.072211	-1.292017	1.176077
	6	-1.087483	-0.965766	0.448557
04	50	1.132293	0.025876	-0.169007
	14	-1.133274	1.185373	0.550805
	14	-2.413617	-0.310165	-0.643480
	6	-1.890897	-1.037778	0.918727
	6	-0.648622	-0.845706	0.626950
05	14	-2.417352	-0.196601	-0.689644
	50	1.237231	-0.082677	-0.094210
	14	-0.912964	1.299084	0.363677
	6	-0.794371	-3.125578	0.000000
	6	0.260752	-2.399953	0.000000
06	14	-1.132771	-1.110088	0.000000
	14	1.361465	-0.939916	0.000000
	50	0.000000	1.237065	0.000000
	14	1.109349	1.321664	-0.285789
	14	1.921412	-0.879072	-0.534120
07	50	-1.084715	-0.075044	-0.067552
	6	0.776392	-0.788227	1.026040
	6	1.191125	0.380877	1.450014
	6	1.056879	1.846690	0.000000
	14	-0.329473	2.925972	0.000000
08	6	0.000000	0.937418	0.000000
	50	-0.521925	-1.178727	0.000000

	14	1.740542	0.090577	0.000000
09	6	0.964865	-0.307310	0.920408
	14	2.121193	-0.387209	-0.645346
	6	1.197005	-1.573934	0.782531
	50	-1.110338	-0.091190	-0.091726
	14	0.917783	1.519136	0.243109
10	14	2.531214	-0.876051	-0.057287
	6	0.990356	-0.211847	0.666918
	6	1.458864	0.601117	-0.408484
	14	0.304486	1.941353	0.042492
	50	-1.087902	-0.344997	-0.026869

$C_2Si_2Sn^-$	Cartesian Coordinates			
01	50	0.000000	0.000000	0.000000
	6	0.000000	0.000000	2.428000
	6	1.270505	0.000000	2.069058
	14	-1.720877	0.000000	2.324274
	14	2.682700	0.000000	1.080179
02	6	0.790976	-1.425681	1.124790
	6	1.078521	-0.152091	1.070278
	14	1.590268	-0.801918	-0.782692
	14	1.314528	1.431296	0.095268
	50	-1.022733	0.007074	-0.065356
03	6	0.304915	1.221894	1.432028
	6	1.076449	0.234460	1.102365
	50	-1.023347	-0.133066	-0.071587
	14	1.821698	-1.112925	0.059725
	14	1.289961	0.979638	-0.850029
04	6	1.352924	-1.037678	1.250632
	6	1.255072	0.228786	0.908328
	14	1.482622	-0.986297	-0.734275
	14	0.995951	1.661187	-0.199769
	50	-0.991383	-0.090651	0.025147
05	14	3.027539	1.154163	0.000000
	6	1.271912	1.459830	0.000000
	14	1.339551	-0.566495	0.000000
	6	0.024528	1.091720	0.000000
	50	-1.364495	-0.480857	0.000000
06	14	-1.798003	1.021089	0.000000
	6	-0.004452	1.142892	0.000000
	50	-0.437316	-1.133155	0.000000
	6	1.262643	1.461554	0.000000
	14	2.895379	1.981606	0.000000
07	14	0.854012	3.331242	0.000000
	14	1.957924	1.276440	0.000000
	6	0.077317	1.709694	0.000000
	6	0.020219	0.396766	0.000000
	50	-0.784949	-1.530672	0.000000
08	6	3.040934	-0.551526	0.443036

	6	2.256060	0.438801	0.2
	14	1.207536	-1.114934	-0.3
	14	0.813700	1.507763	-0.192959
	50	-1.201585	-0.096465	0.062705
	14	1.098802	1.392153	-0.14
	50	-1.130357	-0.085079	-0.036163
09	6	1.953179	-0.486124	1.229881
	6	0.679959	-0.260707	1.151823
	14	1.809700	-0.768230	-0.747622
	14	1.197343	-0.251233	1.712228
	6	1.495242	0.441915	0.000000
10	6	1.197343	-1.004885	0.000000
	14	1.197343	-0.251233	-1.712228
	50	-0.993622	0.208247	0.000000
	6	1.820184	0.548065	0.407843
	14	0.657995	1.772112	-0.293180
11	6	2.546392	-0.456161	0.768109
	14	1.346784	-1.258919	-0.490220
	50	-1.085327	-0.154722	0.078238
	6	-1.511432	1.931038	0.441308
	6	-0.299446	1.762918	0.119932
12	50	-0.710324	-0.541417	-0.068728
	14	1.437315	1.263537	-0.268419
	14	1.875647	-0.913030	0.273345
	6	-0.332332	1.897432	0.860847
	6	0.725007	1.446528	0.315110
13	14	2.100305	0.513021	-0.511733
	14	1.248187	-1.421068	0.495828
	50	-0.984699	-0.147022	-0.136661
	50	-1.272809	-0.000087	0.072348
	14	0.983985	-1.241747	-0.248388
14	14	0.983696	1.242094	-0.248223
	6	2.401639	0.000478	0.083650
	6	3.613851	-0.000562	0.472214
	14	-1.858690	-0.572159	0.000000
	14	0.184808	-1.379826	0.000000
15	50	0.000000	1.254200	0.000000
	6	1.487909	-2.525360	0.000000
	6	2.417817	-3.371672	0.000000
	6	2.147623	-1.660170	-0.241562
	6	0.895271	-1.457085	-0.225851
16	14	1.842738	0.249381	0.265860
	50	-0.989108	-0.246123	0.031698
	14	0.385696	1.965597	-0.178747
	6	1.542553	3.349936	0.000000
	6	1.293971	2.080472	0.000000
17	14	-0.412465	3.082775	0.000000
	14	0.000000	0.743173	0.000000
	50	-0.224893	-1.722915	0.000000
18	6	1.906842	-1.586521	0.598039

	6	0.687240	-1.257147	0.441766
	50	-1.109319	-0.125633	-0.072812
	14	0.713687	1.682126	0.359043
	14	2.136418	-0.014721	-0.544630
19	6	-2.964420	-0.805047	-0.632261
	14	-1.455059	0.168269	-0.001183
	6	-2.982718	-0.776135	0.633344
	50	1.147432	-0.388376	0.001089
	14	-0.094139	1.896437	-0.003172
20	14	0.000000	0.000000	-5.020118
	6	0.000000	0.000000	-3.281414
	6	0.000000	0.000000	-2.010836
	14	0.000000	0.000000	-0.272760
	50	0.000000	0.000000	2.117076

$C_2Si_2Pb^+$			Cartesian Coordinates	
01	82	0.000000	0.000000	0.000000
	6	0.000000	0.000000	2.451000
	6	1.261955	0.000000	2.101159
	14	-1.738928	0.000000	2.662429
	14	2.861539	0.000000	1.387082
02	6	0.845793	-0.703698	-0.000905
	82	-1.308255	-0.310474	-0.000572
	6	2.152511	-0.849342	-0.000778
	14	3.875603	-0.425253	-0.000357
	14	1.752447	1.061768	0.000637
03	6	-0.049808	0.943322	0.000000
	14	1.264706	2.384584	0.000000
	6	-0.674141	2.110622	0.000000
	14	-0.858014	3.867356	0.000000
	82	0.031429	-1.267052	0.000000
04	82	0.000000	1.033604	0.000000
	14	-1.731389	-2.190877	0.000000
	6	-0.000268	-1.240927	0.000000
	6	0.000172	-2.663815	0.000000
	14	1.731430	-2.189629	0.000000
05	82	1.002747	-0.142385	-0.000067
	14	-1.190833	1.818316	0.000190
	6	-1.327049	-0.147121	-0.000194
	6	-2.521210	0.562810	0.000008
	14	-3.033144	-1.162498	0.000279

C_2Si_2Pb	Cartesian Coordinates			
01	82	0.018179	0.000000	0.064894
	6	-0.016660	0.000000	2.441821
	6	1.282771	0.000000	2.077802
	14	-1.728456	0.000000	2.553534
	14	2.803482	0.000000	1.283973

02	6	-0.044515	1.104279	0.000000
	82	-0.611305	-0.947662	0.000000
	14	1.886673	0.796793	0.000000
	6	0.651685	2.256215	0.000000
	14	2.037759	3.316071	0.000000
03	6	2.186930	-0.477248	1.034099
	6	1.689584	0.614834	0.507909
	14	1.752982	-1.331116	-0.537550
	14	0.905430	2.016241	-0.312221
	82	-0.712674	-0.126165	0.040538
04	14	-2.738404	0.250018	-0.710431
	6	-1.476683	0.987575	0.411239
	14	-1.488364	-1.153428	0.613570
	6	-0.521601	1.383389	1.180689
	82	0.867859	-0.019244	-0.099945
05	6	-0.790132	-3.505796	0.000000
	6	0.264385	-2.777085	0.000000
	14	-1.142467	-1.500025	0.000000
	14	1.367787	-1.320942	0.000000
	82	0.000000	0.941352	0.000000
06	6	1.550295	-1.555550	0.810165
	6	1.352944	-0.283082	0.940103
	14	2.436587	-0.433819	-0.673966
	14	1.315333	1.520478	0.227748
	82	-0.853004	-0.050993	-0.051885
07	14	1.462081	1.323192	-0.280477
	14	2.236976	-0.886672	-0.565459
	82	-0.831899	-0.041851	-0.037310
	6	1.155706	-0.808088	1.045802
	6	1.582453	0.361511	1.437958
08	6	-2.296081	-1.026295	0.907134
	14	-1.326926	1.283201	0.378735
	6	-1.041628	-0.859354	0.676183
	82	0.947730	-0.046454	-0.057345
	14	-2.793617	-0.202978	-0.721423
09	6	0.263810	-2.537788	0.000000
	14	1.522815	-1.152636	0.000000
	6	-0.422249	-1.330818	0.000000
	82	0.000000	0.989311	0.000000
	14	-1.454912	-2.983925	0.000000
10	14	2.760109	-1.060578	-0.055435
	6	1.354208	-0.156061	0.682048
	6	1.888616	0.539692	-0.430056
	14	0.845019	1.970360	0.035591
	82	-0.852790	-0.183399	-0.015051

$C_2Si_2Pb^-$	Cartesian Coordinates			
01	82	0.000000	0.000000	0.000000
	6	0.000000	0.000000	2.536000

	6	1.275659	0.000000	2.191801
	14	-1.718252	0.000000	2.490841
	14	2.737984	0.000000	1.288456
	82	-0.785081	0.002671	-0.030311
	14	1.674146	1.425727	0.102085
02	6	1.465602	-0.175450	1.057221
	14	1.906595	-0.777480	-0.821147
	6	1.213464	-1.453159	1.117106
	14	2.051412	-0.706065	0.000000
	82	-0.01823	0.918224	0.000000
03	6	-0.631954	-2.229562	0.000000
	6	0.435238	-1.478948	0.000000
	14	-1.958736	-3.312537	0.000000
	14	0.043807	-3.683932	0.000000
	6	0.977650	-2.155886	0.000000
04	14	-0.932464	-1.452801	0.000000
	6	1.095883	-0.867428	0.000000
	82	0.000000	1.098221	0.000000
	14	1.558772	0.287499	1.714210
	6	1.558772	1.032713	0.000000
05	6	1.824497	-0.408699	0.000000
	14	1.558772	0.287499	-1.714210
	82	-0.779820	-0.143830	0.000000
	82	-0.916978	-0.055737	0.038363
	14	1.576435	-1.121485	-0.345317
06	14	1.220900	1.523295	-0.200560
	6	3.383673	-0.592753	0.469448
	6	2.621241	0.416935	0.279965
	14	1.096009	1.781124	-0.289372
	82	-0.838825	-0.080124	0.045003
07	6	2.175289	0.492948	0.415660
	6	2.860291	-0.541028	0.783767
	14	1.659002	-1.291218	-0.488256
	14	0.088254	-3.662308	0.000000
	14	-0.978831	-1.603151	0.000000
08	6	0.977359	-2.073331	0.000000
	82	0.000000	1.108613	0.000000
	6	1.100653	-0.791641	0.000000
	82	-0.183316	-1.298802	0.000000
	6	0.000000	0.904563	0.000000
09	6	-0.425165	2.146929	0.000000
	14	1.492052	2.358501	0.000000
	14	-0.236131	3.940982	0.000000
	82	-0.866176	-0.044735	-0.018083
	6	1.067229	-0.105866	1.228223
10	14	2.101728	-0.847018	-0.725861
	6	2.298373	-0.496429	1.228717
	14	1.529190	1.367165	-0.221198
11	6	0.171789	2.047298	0.876880
	82	-0.760432	-0.076392	-0.079523

	6	1.141357	1.466005	0.296143
	14	1.490611	-1.464201	0.521904
	14	2.400572	0.405935	-0.558852
	6	-3.998186	-0.001109	0.519564
	6	-2.795093	0.000837	0.104327
12	14	-1.387610	-1.240656	-0.270466
	14	-1.387149	1.241327	-0.270130
	82	0.970808	-0.000095	0.046646
	6	1.426327	3.928479	0.000000
	6	1.229126	2.650050	0.000000
13	14	-0.519722	3.568367	0.000000
	14	0.000000	1.252617	0.000000
	82	-0.105568	-1.304450	0.000000
	14	-1.874500	-0.985481	0.000000
	14	0.176089	-1.770496	0.000000
14	82	0.000000	0.953140	0.000000
	6	1.504562	-2.888352	0.000000
	6	2.458398	-3.707290	0.000000
	6	-0.412421	2.532750	0.450788
	6	0.623347	1.893812	0.109869
15	82	-0.661785	-0.215897	-0.039073
	14	2.030813	0.779410	-0.293893
	14	1.754957	-1.411971	0.282466
	6	-3.348051	-0.835785	-0.611757
	6	-3.138373	-1.112219	0.606958
16	14	-1.835844	0.142822	0.005658
	14	-0.640666	1.985606	0.031084
	82	0.897435	-0.220853	-0.005922
	14	0.000000	0.000000	-5.625643
	6	0.000000	0.000000	-3.888712
17	6	0.000000	0.000000	-2.616314
	14	0.000000	0.000000	-0.879274
	82	0.000000	0.000000	1.586573

S13. Table S11. The low spin states energy (in a.u.) , the high spin states energy (in a.u.) and the energy gap (in kcal/mol) of the isomers in Table S9

$C_3Si_2^+$	the low spin states	the high spin states	the energy gap
01	-691.719366	-691.657337	38.92
02	-691.689750	-691.614915	46.96

C_3Si_2	the low spin states	the high spin states	the energy gap
01	-692.01822	-691.957236	38.27
02	-691.97089	-691.949484	13.43

$C_3Si_2^-$	the low spin states	the high spin states	the energy gap
01	-692.07568	-692.020111	34.87
02	-692.04256	-691.955961	54.34
03	-692.04253	-692.020123	14.06
04	-692.03046	-691.969999	37.94

$C_2Si_3^+$	the low spin states	the high spin states	the energy gap
01	-942.80705	-942.714117	58.31
02	-942.75729	-942.747246	6.30

C_2Si_3	the low spin states	the high spin states	the energy gap
01	-943.08067	-943.050449	18.96
02	-943.05674	-942.983654	45.86
03	-943.05325	----	----
04	-943.04116	-943.026064	9.47

$C_2Si_3^-$	the low spin states	the high spin states	the energy gap
01	-943.13208	-943.079134	33.22
02	-943.12436	-943.089989	21.57
03	-943.12349	----	----
04	-943.11766	----	----
05	-943.11185	-943.034367	48.62
06	-943.10919	-943.074505	21.77
07	-943.106	----	----
08	-943.10562	-943.077303	17.77
09	-943.10008	-943.04252	36.12
10	-943.09519	----	----
11	-943.09413	-943.036707	36.03
12	-943.09169	-943.075705	10.03

$C_2Si_2Ge^+$	the low spin states	the high spin states	the energy gap

01	-2729.3835	-2729.30824	47.22
02	-2729.3808	-2729.30314	48.73
03	-2729.3651	-2729.2903	46.94
04	-2729.3645	----	----

C_2Si_2Ge	the low spin states	the high spin states	the energy gap
01	-2729.6517	-2729.62737	15.26
02	-2729.6494	----	----
03	-2729.6326	----	----
04	-2729.6283	-2729.60028	17.59
05	-2729.625	----	----
06	-2729.6159	-2729.59622	12.35
07	-2729.6142	-2729.60105	8.23
08	-2729.6114	----	----
09	-2729.6097	-2729.59391	9.92

$C_2Si_2Ge^-$	the low spin states	the high spin states	the energy gap
01	-2729.7075	-2729.65494	32.99
02	-2729.7015	-2729.65647	28.26
03	-2729.7006	----	----
04	-2729.6992	----	----
05	-2729.6949	-2729.66484	18.87
06	-2729.6942	----	----
07	-2729.6936	-2729.65161	26.33
08	-2729.6893	-2729.6604	18.15
09	-2729.6873	----	----
10	-2729.6871	----	----
11	-2729.6853	-2729.65687	17.84
12	-2729.6808	-2729.65015	19.26
13	-2729.6805	-2729.64664	21.27
14	-2729.6799	-2729.64679	20.75
15	-2729.6788	-2729.61298	41.28
16	-2729.6776	-2729.64917	17.84
17	-2729.6726	-2729.59759	47.06
18	-2729.6718	-2729.65285	11.92
19	-2729.6689	-2729.63794	19.43
20	-2729.666	----	----
21	-2729.6648	----	----
22	-2729.6629	-2729.63951	14.66
23	-2729.6614	----	----

$C_2Si_2Sn^+$	the low spin states	the high spin states	the energy gap
01	-867.46772	-867.399084	43.07
02	-867.46131	-867.390332	44.54
03	-867.44683	-867.382562	40.33

C_2Si_2Sn	the low spin states	the high spin states	the energy gap
01	-867.72456	-867.702677	13.73
02	-867.71526	-867.698187	10.71
03	-867.70366	----	----
04	-867.70315	----	----
05	-867.69312	----	----
06	-867.69102	-867.658531	20.39
07	-867.68935	----	----
08	-867.68875	-867.663523	15.83
09	-867.68858	-867.683533	3.16
10	-867.68555	----	----

$C_2Si_2Sn^-$	the low spin states	the high spin states	the energy gap
01	-867.78582	-867.731243	34.25
02	-867.77554	----	----
03	-867.77473	----	----
04	-867.77301	----	----
05	-867.76912	-867.742496	16.70
06	-867.76534	----	----
07	-867.76269	----	----
08	-867.76137	-867.741446	12.50
09	-867.76118	-867.743265	11.24
10	-867.76100	-867.705590	34.77
11	-867.76006	----	----
12	-867.75705	-867.722860	21.45
13	-867.75626	-867.725245	19.46
14	-867.75476	----	----
15	-867.75168	-867.699155	32.96
16	-867.75024	-867.719108	19.54
17	-867.74952	-867.722511	16.95
18	-867.74536	-867.720386	15.67
19	-867.74503	-867.684658	37.88
20	-867.74131	-867.719881	13.44

$C_2Si_2Pb^+$	the low spin states	the high spin states	the energy gap
01	-846.10021	-846.033340	41.96
02	-846.09123	-846.022117	43.37
03	-846.08891	-846.035341	33.62
04	-846.07859	-846.019005	37.39
05	-846.07735	----	----

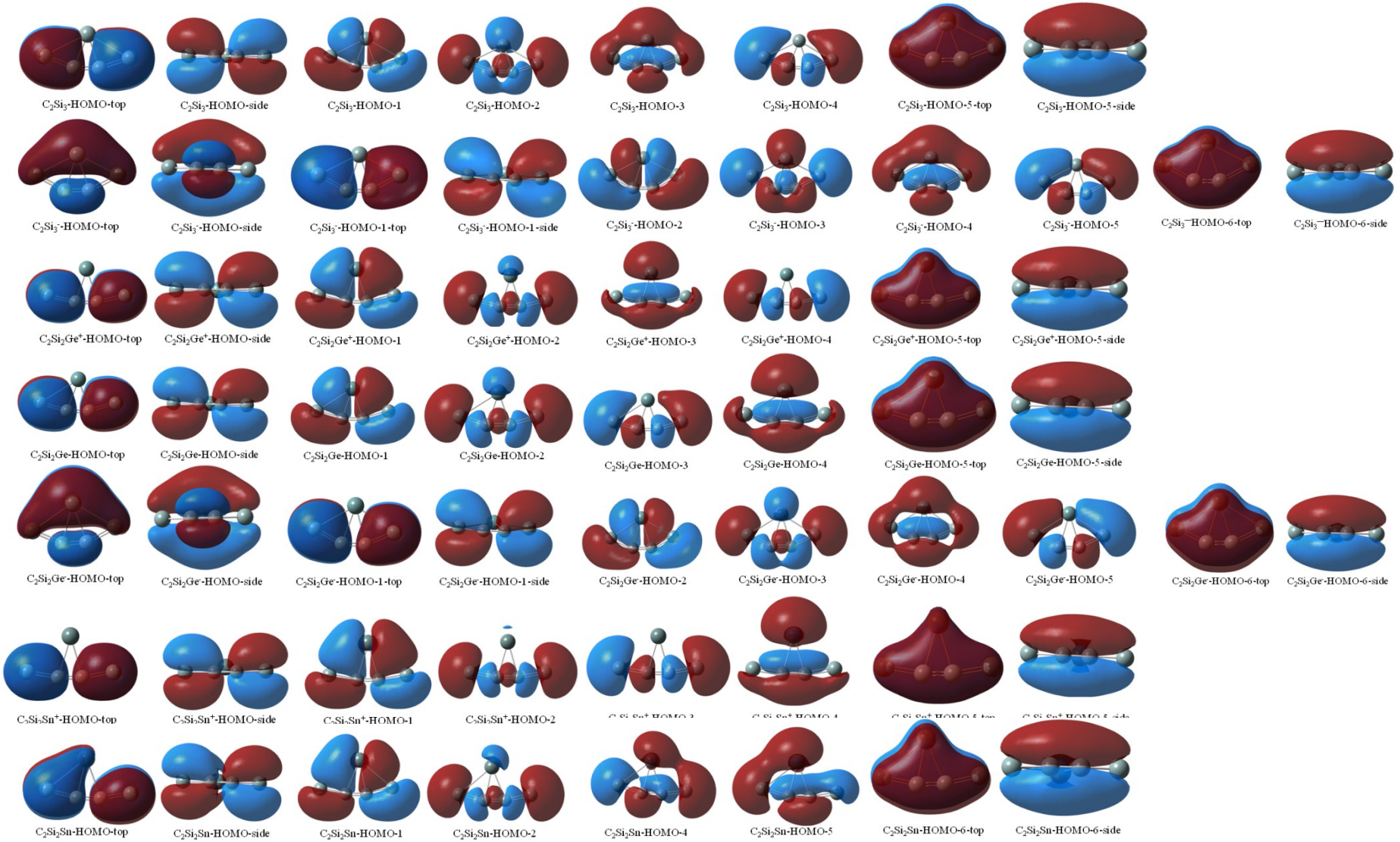
C_2Si_2Pb	the low spin states	the high spin states	the energy gap
01	-846.34805	-846.329513	11.63
02	-846.33663	----	----
03	-846.33042	----	----
04	-846.32969	-846.312261	10.93
05	-846.31933	-846.301952	10.91

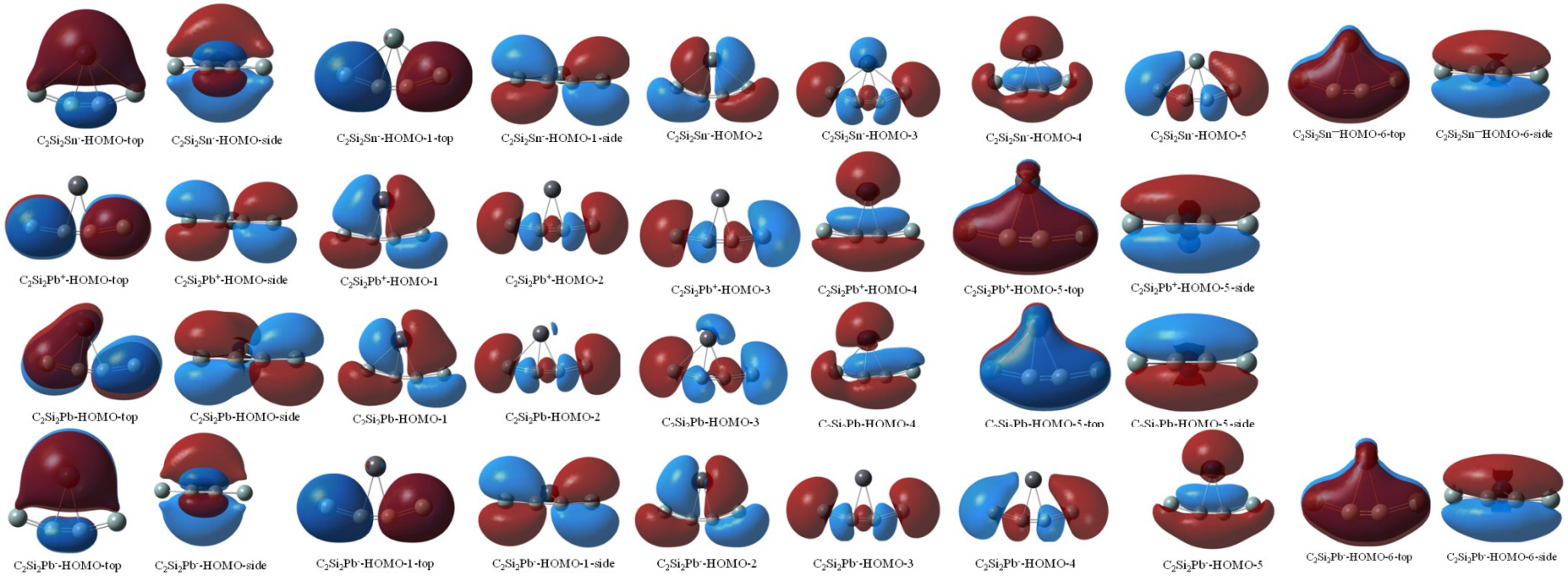
06	-846.31779	----	----
07	-846.31672	----	----
08	-846.3164	----	----
09	-846.31307	-846.301086	7.52
10	-846.31126	----	----

$C_2Si_2Pb^-$	the low spin states	the high spin states	the energy gap
01	-846.41004	-846.356321	33.71
02	-846.40043	----	----
03	-846.38796	----	----
04	-846.38725	-846.368402	11.83
05	-846.38634	-846.334500	32.53
06	-846.38515	----	----
07	-846.38451	----	----
08	-846.38392	----	----
09	-846.38357	----	----
10	-846.38156	-846.367050	9.10
11	-846.37869	-846.348459	18.97
12	-846.37773	-846.368368	5.88
13	-846.37611	-846.351274	15.59
14	-846.37557	-846.313263	39.10
15	-846.37517	-846.345359	18.70
16	-846.36827	-846.321706	29.21
17	-846.36731	----	----

“----”means it does not exit.

S4. Figure S1. Molecular orbitals of global minimum $C_2Si_2X^q$(X= Si, Ge, Sn, Pb; q=0,±1) at the level of B3LYP/def2-TZVPP




$C_2Si_2Sn^-$-HOMO-top
$C_2Si_2Sn^-$-HOMO-side
$C_2Si_2Sn^-$-HOMO-1-top
$C_2Si_2Sn^-$-HOMO-1-side
$C_2Si_2Sn^-$-HOMO-2
$C_2Si_2Sn^-$-HOMO-3
$C_2Si_2Sn^-$-HOMO-4
$C_2Si_2Sn^-$-HOMO-5
$C_2Si_2Sn^-$-HOMO-6-top
$C_2Si_2Sn^-$-HOMO-6-side
$C_2Si_2Pb^+$-HOMO-top
$C_2Si_2Pb^+$-HOMO-side
$C_2Si_2Pb^+$-HOMO-1
$C_2Si_2Pb^+$-HOMO-2
$C_2Si_2Pb^+$-HOMO-3
$C_2Si_2Pb^+$-HOMO-4
$C_2Si_2Pb^+$-HOMO-5-top
$C_2Si_2Pb^+$-HOMO-5-side
C_2Si_2Pb-HOMO-top
C_2Si_2Pb-HOMO-side
C_2Si_2Pb-HOMO-1
C_2Si_2Pb-HOMO-2
C_2Si_2Pb-HOMO-3
C_2Si_2Pb-HOMO-4
C_2Si_2Pb-HOMO-5-top
C_2Si_2Pb-HOMO-5-side
$C_2Si_2Pb^-$-HOMO-top
$C_2Si_2Pb^-$-HOMO-side
$C_2Si_2Pb^-$-HOMO-1-top
$C_2Si_2Pb^-$-HOMO-1-side
$C_2Si_2Pb^-$-HOMO-2
$C_2Si_2Pb^-$-HOMO-3
$C_2Si_2Pb^-$-HOMO-4
$C_2Si_2Pb^-$-HOMO-5
$C_2Si_2Pb^-$-HOMO-6-top
$C_2Si_2Pb^-$-HOMO-6-side

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