Supporting Information

Functionalized Nona-silicide $[Si_9R_3]$ Zintl Clusters: A New Class of Superhalogens

Swapan Sinha[1,2] Puru Jena[3] Santanab Giri[1*]

[1]School of Applied Science and Humanities, Haldia Institute of Technology, Haldia, India. 721657

[2]Maulana Abul Kalam Azad University of Technology, Haringhata, 741249, India.

[3]Physics Department, Virginia Commonwealth University, Richmond, Virginia 23284, United States.

Corresponding Author

* Email: sgiri.chem@hithaldia.in

Table S1: Calculated Laplacian electron density ($\nabla^2\rho$) and energy density (H) values (in atomic units) at BCP (3, -1) of Si-Si bond in $Si_9\{Si\ (^tBu)_2H\}_3]^-$, $[Si_9\{Si\ (TMS)_3\}_3]^-$.

Systems	Si-Si, BCP (3, -1)		Si-Si, BCP (3, -1)		Si-Si, BCP (3, -1)	
	$\nabla^2\rho$	H	$\nabla^2\rho$	H	$\nabla^2\rho$	H
$[Si_9\{Si\ (^tBu)_2H\}_3]^-$	-0.0769	-0.0285	-0.0742	-0.0276	-0.0738	-0.0275
$[Si_9\{Si\ (TMS)_3\}_3]^-$	-0.0699	-0.0275	-0.0699	-0.0275	-0.0696	-0.0274

Table S2: Calculated Laplacian electron density ($\nabla^2\rho$) and energy density (H) values (in atomic units) at BCP (3, -1) of Si-C, Si-C, Si-N bond in $[Si_9(CF_3)_3]^-$, $[Si_9(CN)_3]^-$ and $[Si_9(NO_2)_3]^-$ respectively.

Systems	BCP (3, -1)	$\nabla^2\rho$ (BCP)	H (BCP)
$[Si_9(CF_3)_3]^-$	Si-C	0.2239	-0.0315
	Si-C	0.2715	-0.0314
	Si-C	0.2715	-0.0314
$[Si_9(CN)_3]^-$	Si-C	0.3251	-0.0516
	Si-C	0.3251	-0.0517
	Si-C	0.3251	-0.0517
$[Si_9(NO_2)_3]^-$	Si-N	0.2595	-0.0436
	Si-N	0.2586	-0.0436
	Si-N	0.2597	-0.0436

Table S3: Cartesian coordinates of optimized geometries of $[Si_9(CH_3)_3]^-$.

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.428707	0.099062	-1.592303
2	14	0	-1.427782	0.098986	1.593146
3	14	0	-1.304118	-1.862785	0.000074
4	14	0	0.659540	-1.347938	1.491203
5	14	0	0.659279	-1.347292	-1.492001
6	14	0	2.300002	-0.154665	-0.000027
7	14	0	0.835014	1.233396	-1.507746
8	14	0	-1.024125	2.024124	0.000088
9	14	0	0.835222	1.233751	1.507293
10	6	0	4.236100	-0.277650	0.000179
11	1	0	4.559356	-0.816380	-0.865948
12	1	0	4.655997	0.706407	-0.014568
13	1	0	4.560795	-0.790811	0.881167
14	6	0	-2.455130	-3.424442	0.000132
15	1	0	-3.478808	-3.113021	0.000456
16	1	0	-2.260942	-4.010675	-0.873666
17	1	0	-2.260475	-4.010956	0.873637
18	6	0	-1.935512	3.736717	0.000098
19	1	0	-1.658670	4.288076	-0.874122
20	1	0	-2.993622	3.577650	0.001244
21	1	0	-1.656918	4.288998	0.873179

Table S4: Cartesian coordinates of optimized geometries of $[Si_9(CF_3)_3]^-$.

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.373798	0.515138	-1.696207
2	14	0	-1.378925	0.525404	1.666382
3	14	0	-1.483836	-1.229287	-0.006341
4	14	0	0.234934	-1.475378	1.687842
5	14	0	0.235307	-1.479166	-1.707375
6	14	0	1.796711	-0.713570	-0.006328
7	14	0	1.161104	0.910735	-1.700010
8	14	0	-0.288672	1.889819	-0.013082
9	14	0	1.163655	0.922435	1.669762
10	6	0	3.640739	-1.369105	0.009544
11	6	0	-3.043275	-2.411591	0.009466
12	6	0	-0.616803	3.818979	0.005990
13	9	0	-0.490362	4.352745	1.254627
14	9	0	0.241946	4.520496	-0.788679
15	9	0	-1.868360	4.160065	-0.417208
16	9	0	4.565984	-0.389148	-0.205260
17	9	0	3.881307	-2.314189	-0.944485
18	9	0	3.982115	-1.943242	1.198958
19	9	0	-4.221037	-1.756868	-0.206135
20	9	0	-3.195611	-3.061152	1.199165
21	9	0	-2.986503	-3.385987	-0.943760

Table S5: Cartesian coordinates of optimized geometries of $[Si_9(CN)_3]^-$.

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.415080	0.357412	1.669279
2	14	0	1.418737	0.361772	-1.658607
3	14	0	1.397377	-1.415715	-0.000264
4	14	0	-0.402615	-1.426560	-1.632291
5	14	0	-0.401455	-1.425809	1.639619
6	14	0	-1.936082	-0.487275	0.000697
7	14	0	-1.029671	1.048885	1.652777
8	14	0	0.547149	1.907135	0.003361
9	14	0	-1.032125	1.055128	-1.640532
10	6	0	1.085727	3.770844	-0.007739
11	7	0	1.407763	4.885226	-0.014376
12	6	0	-3.820346	-0.948844	-0.009400
13	7	0	-4.947019	-1.224834	-0.015438
14	6	0	2.755905	-2.800602	-0.009666
15	7	0	3.568221	-3.628679	-0.015288

Table S6: Cartesian coordinates of optimized geometries of $[Si_9(NO_2)_3]^-$.

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.415619	0.351412	1.670360
2	14	0	1.419244	0.352296	-1.657528
3	14	0	1.389635	-1.423348	0.002661
4	14	0	-0.410414	-1.427509	-1.629334
5	14	0	-0.409200	-1.423363	1.642573
6	14	0	-1.939465	-0.479397	0.002693
7	14	0	-1.025887	1.054242	1.653166
8	14	0	0.554886	1.903426	0.002842
9	14	0	-1.028363	1.057074	-1.640148
10	7	0	1.082390	3.697439	-0.009730
11	7	0	-3.757793	-0.915861	-0.006558
12	7	0	2.692914	-2.764357	-0.005029
13	8	0	2.404172	4.017575	-0.011884
14	8	0	-4.693965	0.070377	0.016200
15	8	0	-4.144041	-2.219526	-0.036045
16	8	0	0.144246	4.682039	-0.016720
17	8	0	4.011464	-2.431156	-0.003305
18	8	0	2.322203	-4.072837	-0.012344

Table S7: Cartesian coordinates of optimized geometries of $[Si_9\{Si(^tBu)_2H\}_3]^-$.

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.400080	0.958405	1.398795
2	14	0	-0.917918	1.172531	-1.887012
3	14	0	1.411469	0.174868	-1.579157
4	14	0	0.930990	-0.033196	1.650587
5	14	0	0.911209	-1.701970	-0.120513
6	14	0	-1.080158	-1.558626	1.266803
7	14	0	-2.230453	-0.327484	-0.495195
8	14	0	-0.602409	-1.353060	-1.985185
9	14	0	-4.103435	-0.538803	-0.797895
10	6	0	-6.378866	-3.159631	-0.329631
11	1	0	-6.923993	-3.761641	0.367019
12	1	0	-7.044119	-2.463791	-0.796692
13	1	0	-5.938448	-3.787717	-1.075579
14	6	0	-5.725360	-1.361186	2.195204
15	1	0	-6.603743	-0.809691	1.932154
16	1	0	-5.979474	-2.118215	2.907408
17	1	0	-5.002384	-0.697986	2.622254
18	6	0	-3.573458	-3.421859	1.118536
19	1	0	-2.910994	-3.569511	0.291348
20	1	0	-3.027754	-3.015639	1.944425
21	1	0	-4.004276	-4.359317	1.402207
22	6	0	-7.000360	1.380804	-1.232100
23	1	0	-7.685461	1.987260	-0.677349
24	1	0	-6.938396	1.741319	-2.237629
25	1	0	-7.344224	0.367574	-1.237031
26	6	0	-5.445041	1.733007	1.505271
27	1	0	-5.318131	2.770360	1.734819
28	1	0	-6.420589	1.416883	1.810675
29	1	0	-4.705571	1.159775	2.024396
30	6	0	-4.244098	2.941214	-1.165729
31	1	0	-3.505912	3.269447	-0.464127
32	1	0	-3.762799	2.619746	-2.065679
33	1	0	-4.910377	3.748828	-1.386482
34	6	0	2.434027	-2.110076	-2.996789
35	1	0	1.367828	-2.200128	-2.999781
36	1	0	2.705794	-1.096808	-2.786239
37	1	0	2.818352	-2.390648	-3.955160
38	6	0	3.274254	-5.088403	-2.318664
39	1	0	2.476546	-5.250924	-3.013034
40	1	0	4.212227	-5.233927	-2.812556
41	1	0	3.187302	-5.780400	-1.507196
42	6	0	4.958206	-2.665745	-1.164844
43	1	0	5.474013	-3.442599	-0.640114
44	1	0	5.497338	-2.417956	-2.055258
45	1	0	4.885357	-1.800514	-0.539569
46	6	0	3.798363	-1.364438	1.796370
47	1	0	3.677481	-0.799905	0.895487
48	1	0	3.225901	-0.913112	2.579627
49	1	0	4.832001	-1.378327	2.072593
50	6	0	4.708148	-4.348147	1.243161
51	1	0	5.596199	-3.758368	1.151362
52	1	0	4.802932	-5.007626	2.080421
53	1	0	4.567397	-4.922129	0.351178
54	6	0	2.175138	-3.775051	3.057461

55	1	0	2.678946	-4.600765	3.514926
56	1	0	2.095278	-2.972208	3.760288
57	1	0	1.196200	-4.079775	2.751317
58	6	0	3.850317	2.407070	1.588882
59	1	0	3.834545	1.634820	2.329342
60	1	0	3.819033	1.967146	0.614004
61	1	0	4.746827	2.981964	1.692154
62	6	0	1.293805	2.975613	3.371373
63	1	0	0.249053	3.001605	3.141767
64	1	0	1.578124	1.976166	3.626653
65	1	0	1.493658	3.625367	4.197677
66	6	0	2.907353	5.387821	2.100947
67	1	0	2.105731	5.967989	2.508016
68	1	0	3.733503	5.394439	2.780898
69	1	0	3.212194	5.807777	1.165207
70	6	0	3.967612	4.670664	-0.702293
71	1	0	4.611581	4.811037	-1.545204
72	1	0	3.796320	5.612163	-0.223609
73	1	0	4.427973	3.997093	-0.010000
74	6	0	2.602905	2.332217	-2.347136
75	1	0	2.980998	1.558980	-1.711487
76	1	0	1.688092	2.008099	-2.797652
77	1	0	3.319965	2.548113	-3.111409
78	6	0	1.343961	5.239095	-2.384437
79	1	0	1.233676	6.148566	-1.831627
80	1	0	1.906500	5.428787	-3.274643
81	1	0	0.377680	4.861747	-2.646756
82	14	0	1.189253	3.479542	0.245450
83	14	0	2.043874	-3.236750	-0.061716
84	1	0	-4.315835	-0.941228	-2.195693
85	1	0	0.092284	4.449906	0.371755
86	1	0	1.218175	-4.452366	-0.024316
87	6	0	-5.247108	1.464674	-0.405859
88	6	0	-4.982862	-2.190975	0.606574
89	6	0	2.310182	3.562511	1.826663
90	6	0	2.275933	3.930380	-1.297104
91	6	0	3.177590	-3.275244	-1.635503
92	6	0	3.181381	-3.181097	1.508819
93	14	0	0.465325	1.726041	0.033999

Table S8: Cartesian coordinates of optimized geometries of $[Si_9\{Si(TMS)_3\}_3]^-$.

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.356374	0.484737	-1.685341
2	14	0	1.361805	0.483038	1.642545
3	14	0	0.385035	1.968244	-0.015798
4	14	0	-1.136493	1.006452	1.616229
5	14	0	-1.135111	1.006446	-1.655681
6	14	0	-1.921089	-0.611629	-0.016759
7	14	0	-0.329237	-1.416225	-1.668839
8	14	0	1.461463	-1.288368	-0.019423
9	14	0	-0.327936	-1.422806	1.624470
10	14	0	2.896965	-2.546763	-0.008500
11	14	0	4.940884	-1.490376	-0.435167
12	14	0	2.554884	-4.199595	-1.629217

13	14	0	3.019101	-3.583372	2.085808
14	14	0	-3.809075	-3.143324	-0.311198
15	14	0	-4.542302	-0.842122	1.710372
16	14	0	-4.757084	-0.336216	-1.386976
17	14	0	2.667350	4.155208	-0.295225
18	14	0	0.274906	4.602414	1.704163
19	14	0	-0.226493	4.744127	-1.397923
20	6	0	3.222231	-5.898276	-0.971393
21	1	0	3.265576	-6.600705	-1.777379
22	1	0	4.202046	-5.762673	-0.563380
23	1	0	2.567144	-6.268349	-0.210599
24	6	0	3.500708	-3.718397	-3.253245
25	1	0	4.555147	-3.792153	-3.087059
26	1	0	3.216547	-4.383425	-4.041845
27	1	0	3.252094	-2.714210	-3.526556
28	6	0	0.658106	-4.352411	-2.006685
29	1	0	0.102404	-4.216240	-1.102499
30	1	0	0.374141	-3.603398	-2.716083
31	1	0	0.451613	-5.321878	-2.409665
32	6	0	2.098342	-5.289578	2.017522
33	1	0	2.798259	-6.063331	1.780198
34	1	0	1.651636	-5.492110	2.968487
35	1	0	1.337289	-5.254344	1.266218
36	6	0	4.878780	-3.870564	2.557735
37	1	0	5.338379	-2.931267	2.784431
38	1	0	4.934884	-4.510783	3.413230
39	1	0	5.388775	-4.328040	1.735835
40	6	0	2.181439	-2.449384	3.418473
41	1	0	2.459930	-1.430765	3.245970
42	1	0	1.117881	-2.544800	3.350361
43	1	0	2.504498	-2.747142	4.394113
44	6	0	6.395415	-2.648684	0.118244
45	1	0	7.254239	-2.458690	-0.491037
46	1	0	6.635229	-2.455330	1.142941
47	1	0	6.099017	-3.670891	0.008060
48	6	0	5.094342	-1.121627	-2.333607
49	1	0	5.562817	-0.170140	-2.475398
50	1	0	5.685442	-1.882986	-2.798185
51	1	0	4.119406	-1.108372	-2.774315
52	6	0	5.027426	0.174989	0.556129
53	1	0	4.552197	0.950580	-0.007357
54	1	0	4.526781	0.057928	1.494506
55	1	0	6.051031	0.434986	0.727984
56	6	0	-2.351609	-3.676239	-1.475412
57	1	0	-2.231375	-2.949788	-2.251758
58	1	0	-1.447563	-3.743810	-0.907051
59	1	0	-2.572031	-4.629047	-1.909545
60	6	0	-3.656528	-4.074766	1.383719
61	1	0	-4.634124	-4.292100	1.760509
62	1	0	-3.117891	-4.988292	1.241451
63	1	0	-3.133431	-3.457638	2.084022
64	6	0	-5.501377	-3.593172	-1.146274
65	1	0	-5.649314	-4.652078	-1.104639
66	1	0	-6.297201	-3.101173	-0.627139
67	1	0	-5.490998	-3.274378	-2.167627
68	6	0	-3.155394	-0.487153	3.019602
69	1	0	-2.335276	-1.155753	2.860605
70	1	0	-2.817416	0.522792	2.916250
71	1	0	-3.548547	-0.632716	4.004052
72	6	0	-5.597585	-2.365890	2.283180
73	1	0	-4.979832	-3.037968	2.841386

74	1	0	-6.405327	-2.029142	2.898853
75	1	0	-5.989631	-2.870989	1.425232
76	6	0	-5.689443	0.713672	1.545533
77	1	0	-6.598208	0.436224	1.053527
78	1	0	-5.913532	1.096363	2.519305
79	1	0	-5.189291	1.466521	0.972849
80	6	0	-4.249556	1.534614	-1.464484
81	1	0	-3.752823	1.807314	-0.556854
82	1	0	-3.590519	1.691367	-2.292735
83	1	0	-5.125400	2.137012	-1.586612
84	6	0	-6.647733	-0.476842	-0.975549
85	1	0	-7.029312	0.488841	-0.717181
86	1	0	-7.171912	-0.850485	-1.830257
87	1	0	-6.784753	-1.146443	-0.152287
88	6	0	-4.404261	-1.173521	-3.101047
89	1	0	-5.325407	-1.506802	-3.531529
90	1	0	-3.940502	-0.465152	-3.755295
91	1	0	-3.752277	-2.010420	-2.961706
92	6	0	-2.123797	4.624244	-1.011315
93	1	0	-2.613778	4.083468	-1.793863
94	1	0	-2.266824	4.114218	-0.081629
95	1	0	-2.537241	5.608925	-0.945222
96	6	0	0.138967	3.906418	-3.109146
97	1	0	1.026859	3.314063	-3.033891
98	1	0	-0.684837	3.281042	-3.383287
99	1	0	0.276446	4.662114	-3.854077
100	6	0	0.303276	6.609197	-1.464684
101	1	0	1.254787	6.692656	-1.946931
102	1	0	-0.425403	7.167494	-2.014440
103	1	0	0.372636	6.996115	-0.469504
104	6	0	-0.735460	6.232582	1.412085
105	1	0	-1.110477	6.592197	2.347468
106	1	0	-0.099003	6.973116	0.974555
107	1	0	-1.554164	6.031548	0.753140
108	6	0	-0.815002	3.333346	2.686592
109	1	0	-1.618536	2.997131	2.065148
110	1	0	-0.214292	2.496722	2.976606
111	1	0	-1.213312	3.806234	3.559876
112	6	0	1.874505	5.007078	2.724521
113	1	0	2.436591	5.765454	2.220710
114	1	0	1.598143	5.355267	3.697808
115	1	0	2.471034	4.123704	2.817819
116	6	0	3.285821	3.073255	-1.781990
117	1	0	3.703154	2.160965	-1.409886
118	1	0	2.462504	2.851309	-2.428357
119	1	0	4.032920	3.610742	-2.327746
120	6	0	3.654854	3.679602	1.305473
121	1	0	4.537564	3.139813	1.032795
122	1	0	3.929430	4.569288	1.832698
123	1	0	3.042223	3.067385	1.933783
124	6	0	2.953141	6.031329	-0.697836
125	1	0	3.968603	6.291502	-0.483250
126	1	0	2.750702	6.208742	-1.733424
127	1	0	2.297747	6.628509	-0.098892
128	14	0	0.775582	3.836648	-0.006547
129	14	0	-3.726787	-1.229117	-0.006826

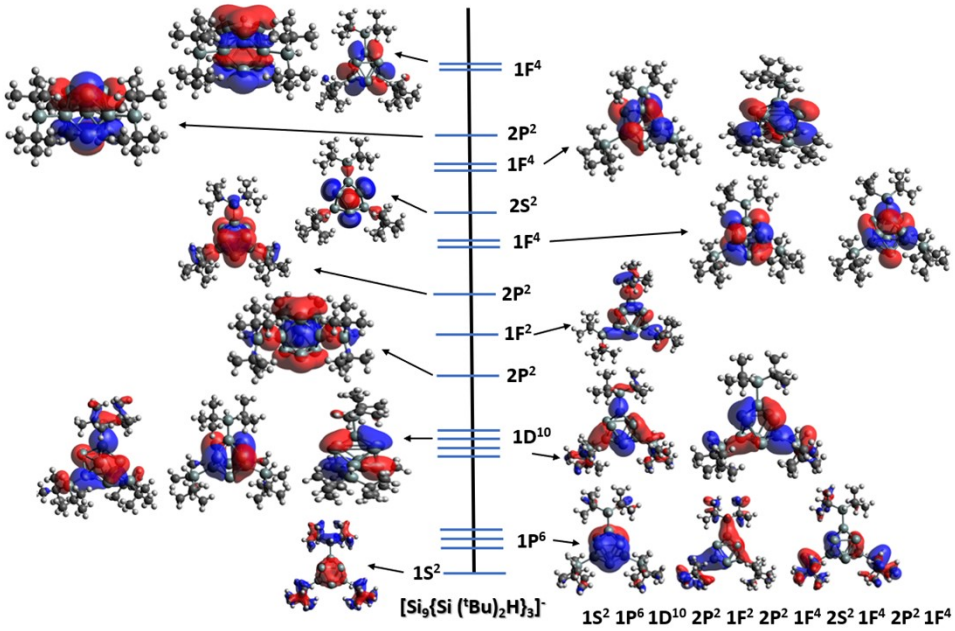

Fig S1: Electron shell structures of the $[Si_9\{Si\ (^tBu)_2H\}_3]^-$.

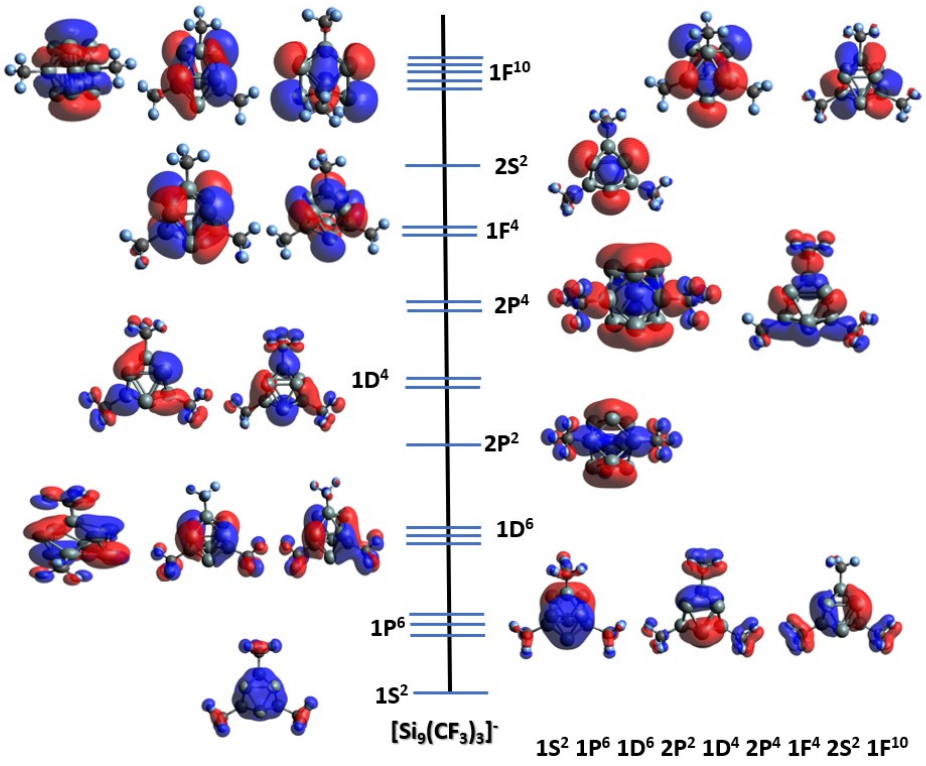

Fig S2: Electron shell structures of the $[Si_9(CF_3)_3]^-$.

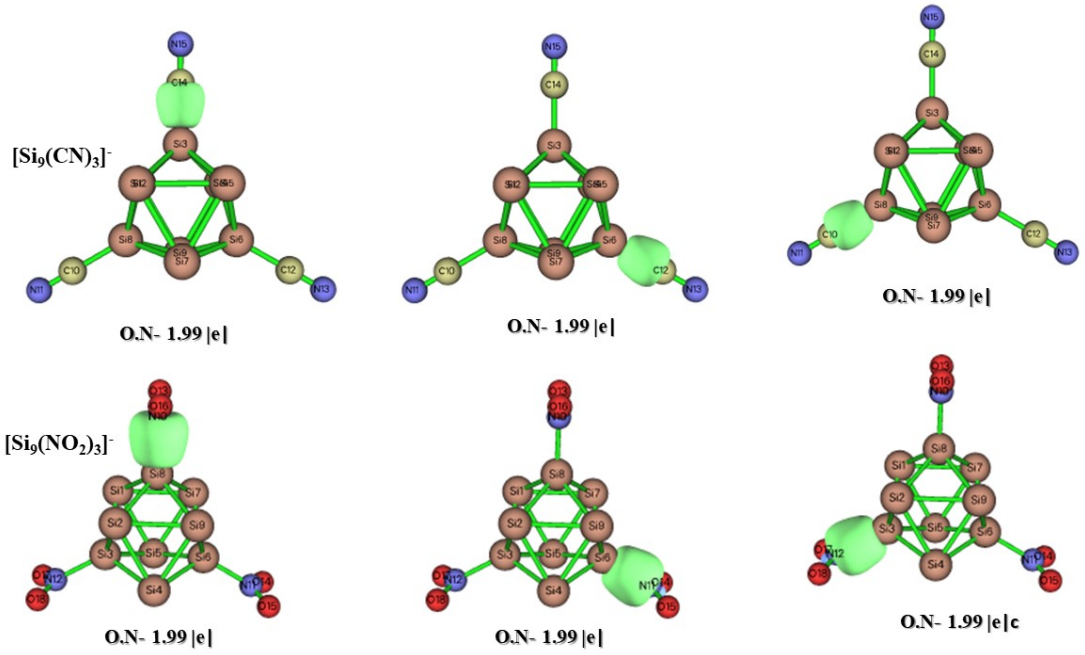

Fig. S3: AdNDP 2c-2e bond study $[Si_9(CN)_3]^-$, $[Si_9(NO_2)_3]^-$.

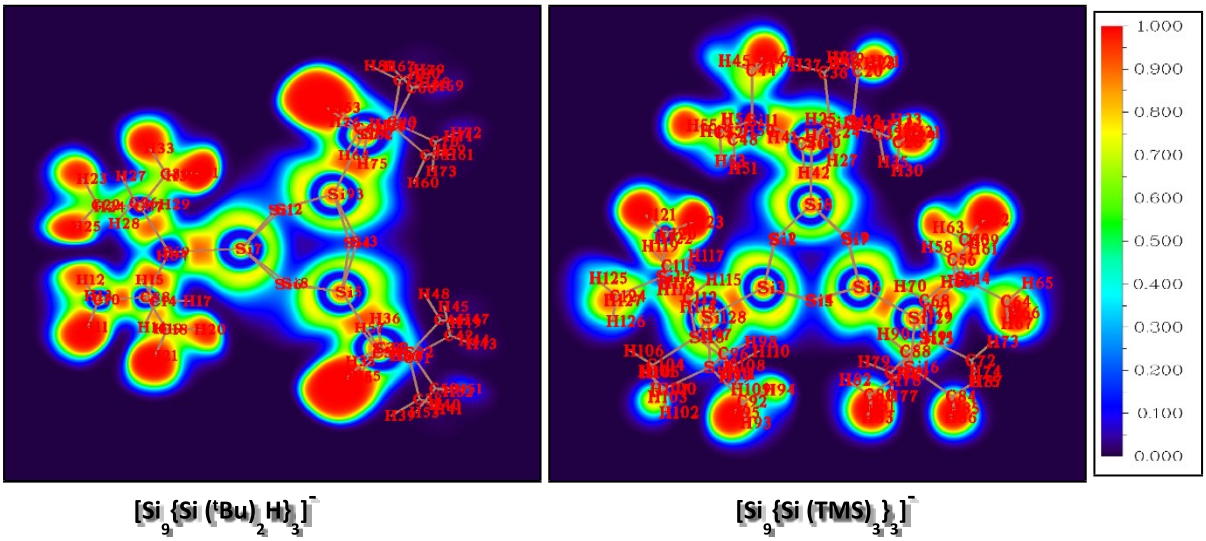

Fig. S4: Cut of plane ELF plot of $[Si_9\{Si\ (^tBu)_2H\}_3]^-$ and $[Si_9\{Si\ (TMS)_3\}_3]^-$.

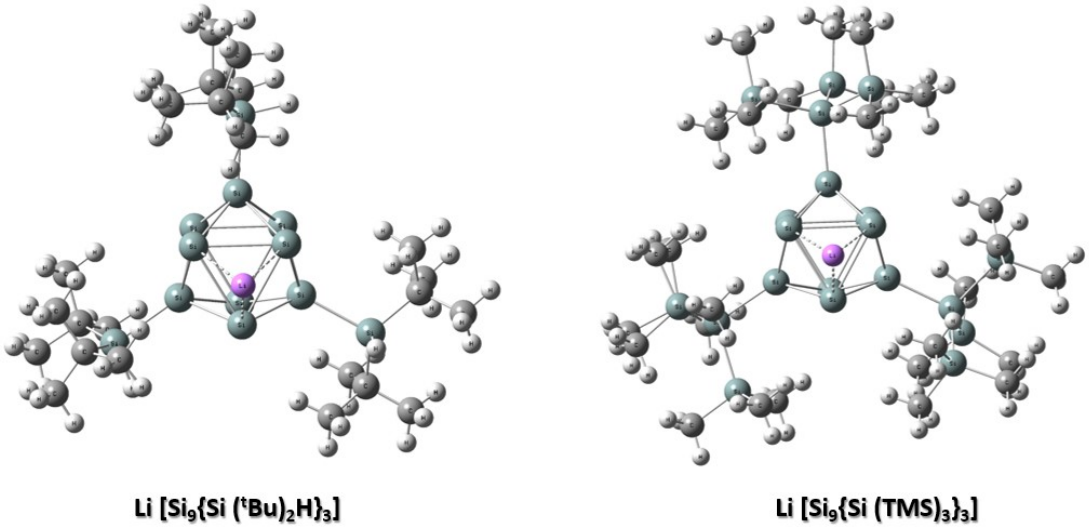

Fig. S5: Ground state geometries of different Li-Salts containing proposed electrolytes in Li-ion batteries.

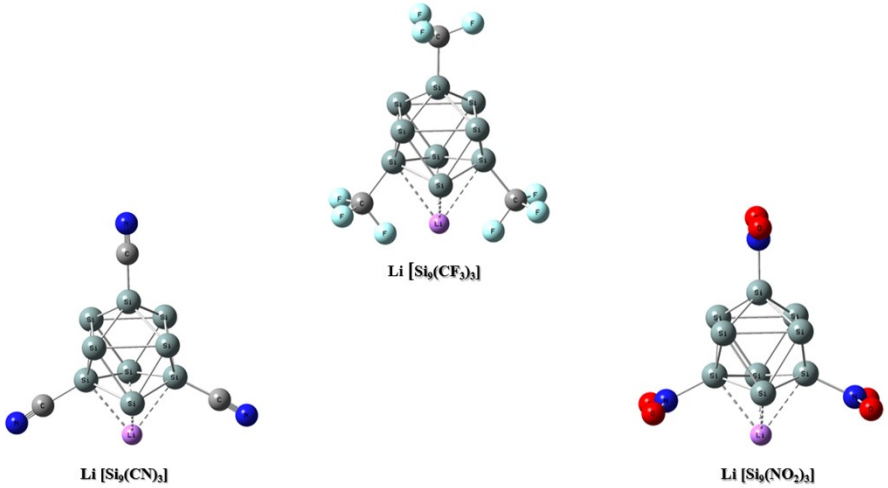

Fig. S6: Ground state geometries of different Li-Salts containing proposed electrolytes in Li-ion batteries.