Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Materials

How are small endohedral silicon clusters stabilized?

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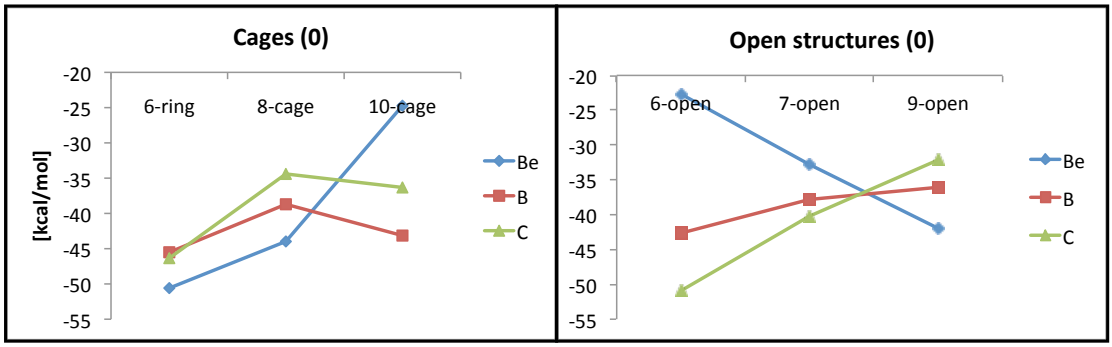

Figure S1: $\Delta E_{cage\ relaxation}$ [kcal/mol] towards the neutral ring/cage and open structures of XSi_n (n=6-10) after removal of the interstitial atom. Energies are computed at the B3LYP/aug-cc-pVTZ level.

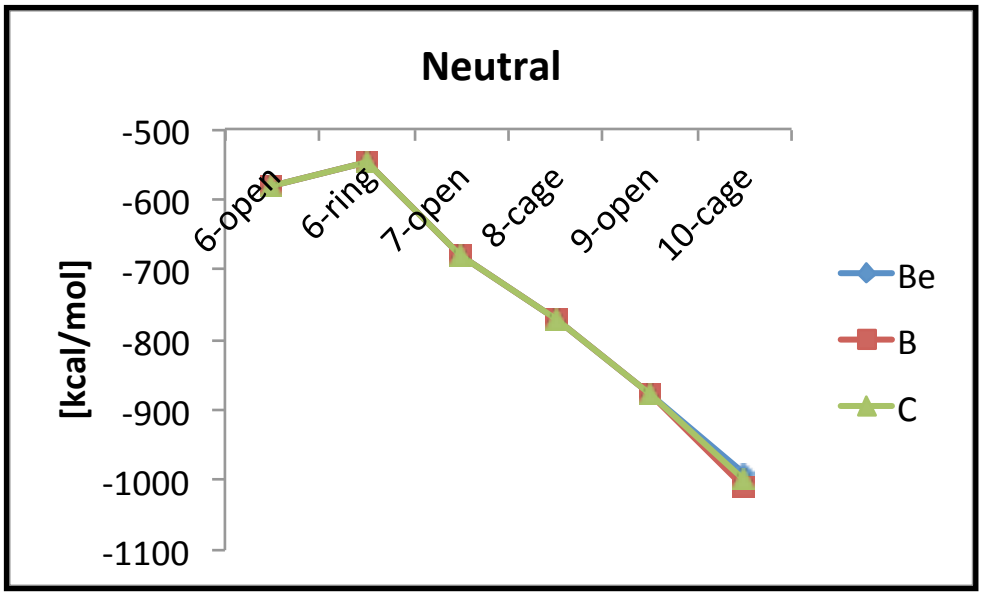

Figure S2: $\Delta E_{Si(n)\ atomisation}$ [kcal/mol] of the neutral ring, cages and open structures of XSi_n (n=6-10). Energies are computed at the B3LYP/aug-cc-pVTZ level.

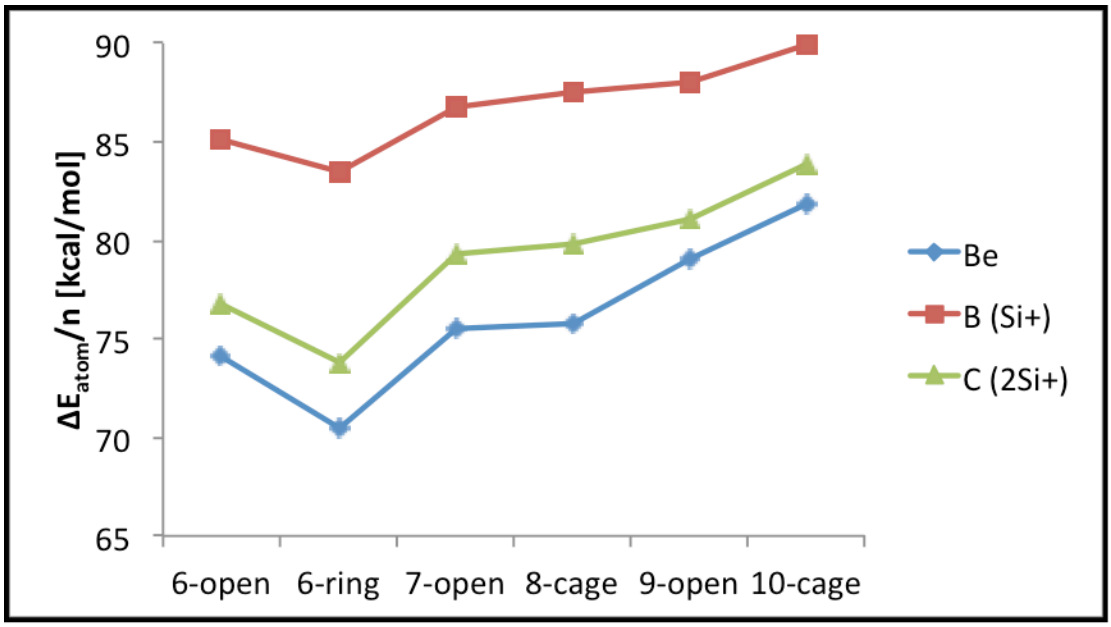

Figure S3: Atomization energy per atom [kcal/mol] of the bordered structures of Fig. 3 and Fig. S4, computed at the CCSD(T)-F12b level. For the charged clusters, the lowest-energy fragmentation produces singly-charged Si atoms through XSi_n^{a+} -> X + aSi^+ + (n-a)Si.

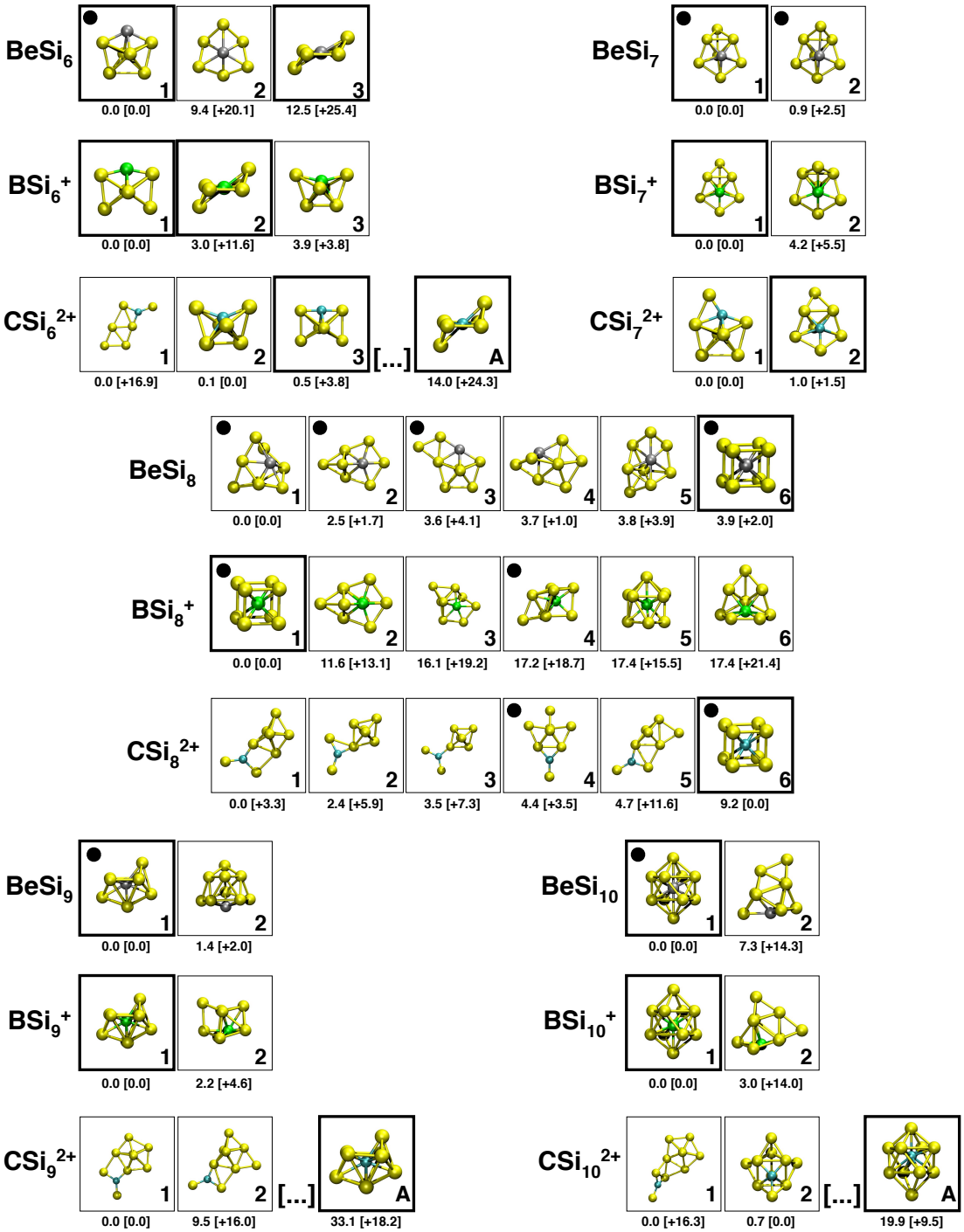

Figure S4: XSi_{6-10} low-lying singlet isomers. Values in bold are relative energies in kcal/mol at the CCSD(T)-F12b/VDZ-F12 and B3LYP/aug-cc-pVTZ level (within brackets). Black dots (upper left corner) indicate structures previously described in the literature. Bordered structures are the symmetric isomers further analyzed in this work. T1 diagnostics are given in Table S1.

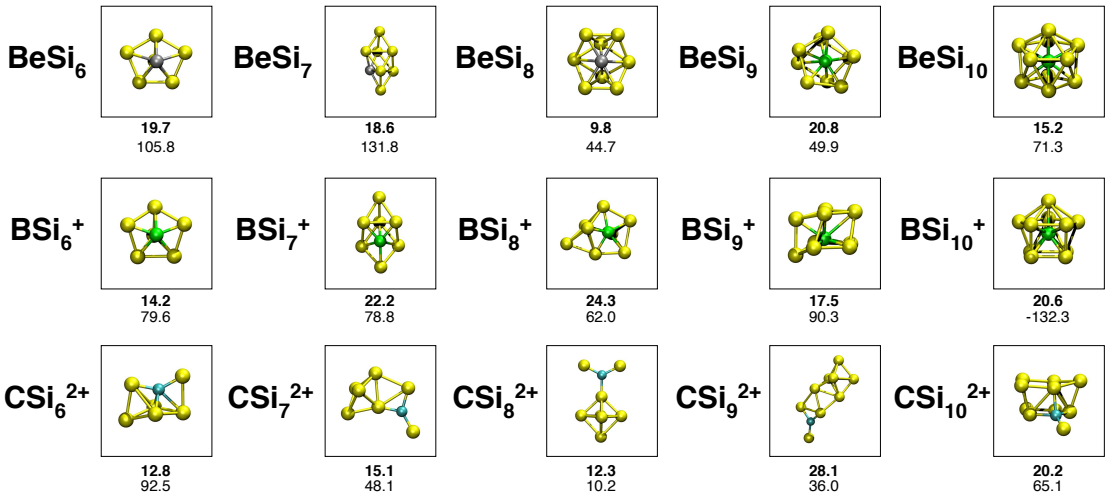

Figure S5: Lowest-lying triplet structures located for XSi_{6-10}, along with relative B3LYP/aug-cc-pVTZ energies [kcal/mol] and vibrational frequencies [cm^{-1}] computed at the same level.

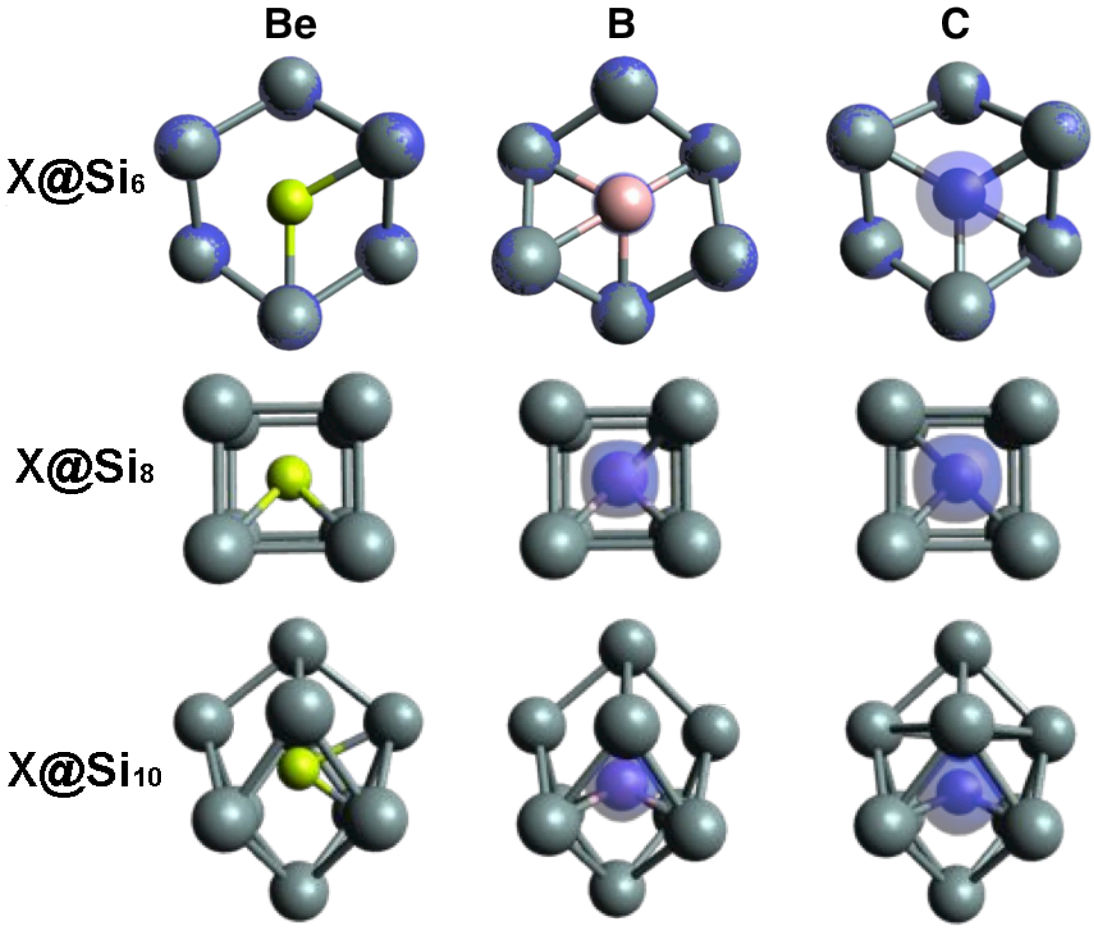

Fig. S6: B3LYP/ aug-cc-pVTZ electron density for the endohedral $X@Si_{6-10}$ isomers. Isovalue is 0.08 (0.06 for $X@Si_6$).

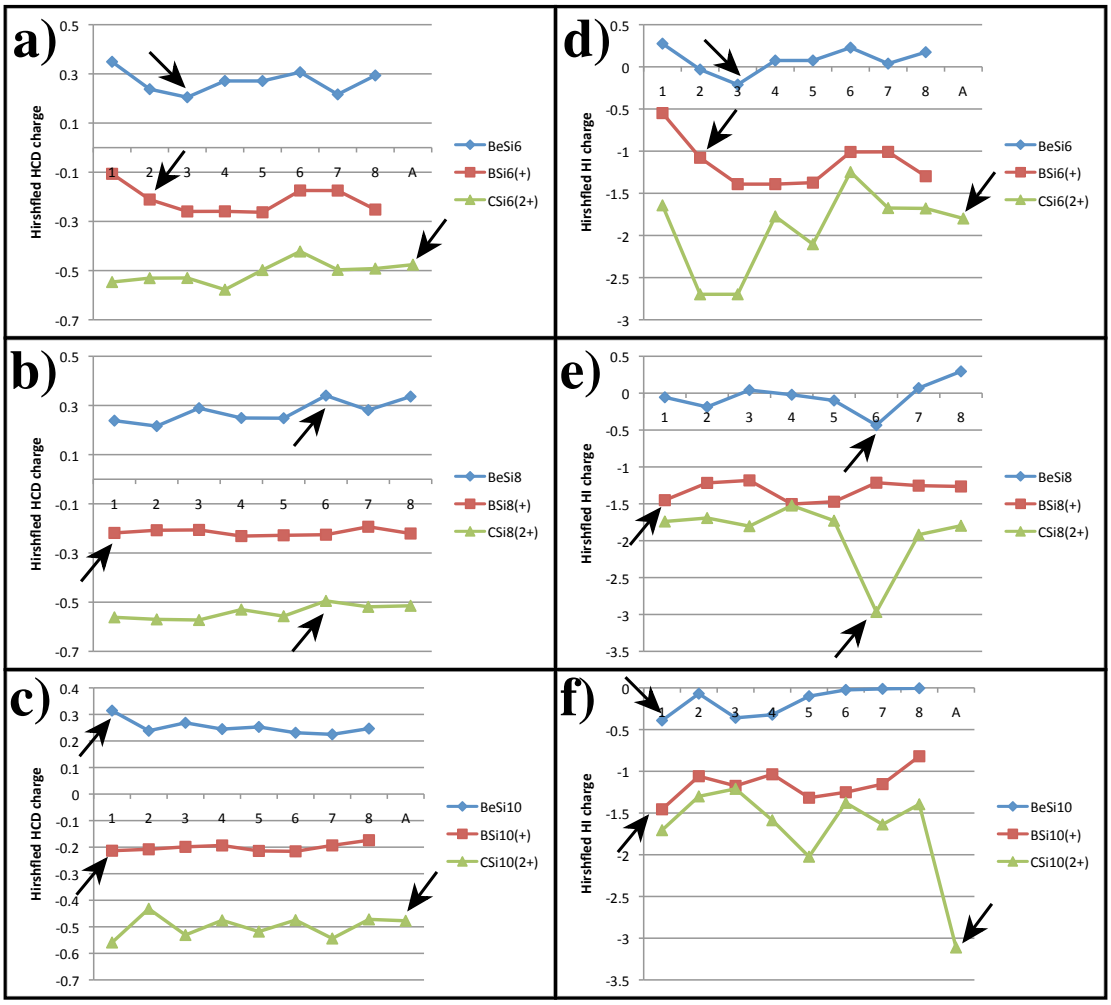

Figure S7: Hirshfeld classical dominant (left) and Hirshfeld iterative (right) charges for low-lying isomers shown in Figure S4, a,d) XSi_6, b, e) XSi_8 and c, f) XSi_{10}. Arrows refer to the $X@Si_6$ rings, the $X@Si_8$ and $X@Si_{10}$ cages.

Table S1: T1 diagnostics for the XSi_n structures. The number or symbol in parenthesis refers to the molecule label as used in Figure S4.

n=	$BeSi_n$	BSi_n^+	CSi_n^{2+}
6 (**1**)	0.021	0.025	0.022
6 (**2**)	0.030	0.032	0.023
6 (**3**)	0.042	0.021	0.032
6 (**A**)			0.029
7 (**1**)	0.024	0.022	0.023
7 (**2**)	0.028	0.024	0.021
8 (**1**)	0.028	0.017	0.024
8 (**2**)	0.026	0.023	0.025
8 (**3**)	0.022	0.026	0.025
8 (**4**)	0.025	0.023	0.022
8 (**5**)	0.028	0.021	0.028
8 (**6**)	0.016	0.026	0.018

9 (**1**)	0.029	0.022	0.023
9 (**2**)	0.030	0.031	0.026
9 (**A**)			0.019
10 (**1**)	0.024	0.021	0.024
10 (**2**)	0.027	0.025	0.028
10 (**A**)			0.021

Table S2: Charge of the X atoms in the isomers of XSi_{6-10} shown in Figure S4 using Mulliken, NPA and Hirshfeld classical (HC), and iterative dominant (HID) schemes, and Voronoi deformation density (VDD). Values were computed at the B3LYP/aug-cc-pVTZ level, except for the VDD charges, which were computed at the B3LYP/ATZ2P level (in ADF 2012).

	Compound	Mulliken	NPA	HC	HCD	HI	HID	VDD
XSi_6	$BeSi_6$ **1**	1.29	-0.11	0.09	0.35	0.28	0.48	0.02
	BSi_6^+ **1**	0.46	-1.20	-0.10	-0.11	-0.55	-0.32	-0.23
	CSi_6^{2+} **3**	0.19	-1.98	-0.29	-0.53	-2.70	-2.53	-0.34
XSi_7	$BeSi_7$ **1**	1.82	-0.63	-0.03	0.23	-0.05	-0.77	-0.12
	BSi_7^+ **1**	0.85	-1.72	-0.17	-0.20	-0.96	-0.51	-0.34
	CSi_7^{2+} **2**	0.28	-2.24	-0.22	-0.48	-1.57	-1.99	-0.39
XSi_9	$BeSi_9$ **1**	4.25	-2.16	-0.16	0.27	-0.37	-0.79	-0.31
	BSi_9^+ **1**	3.41	-2.47	-0.20	-0.21	-1.39	-1.56	-0.40
	CSi_9^{2+} **A**	1.79	-2.92	-0.20	-0.47	-2.95	-3.05	-0.41

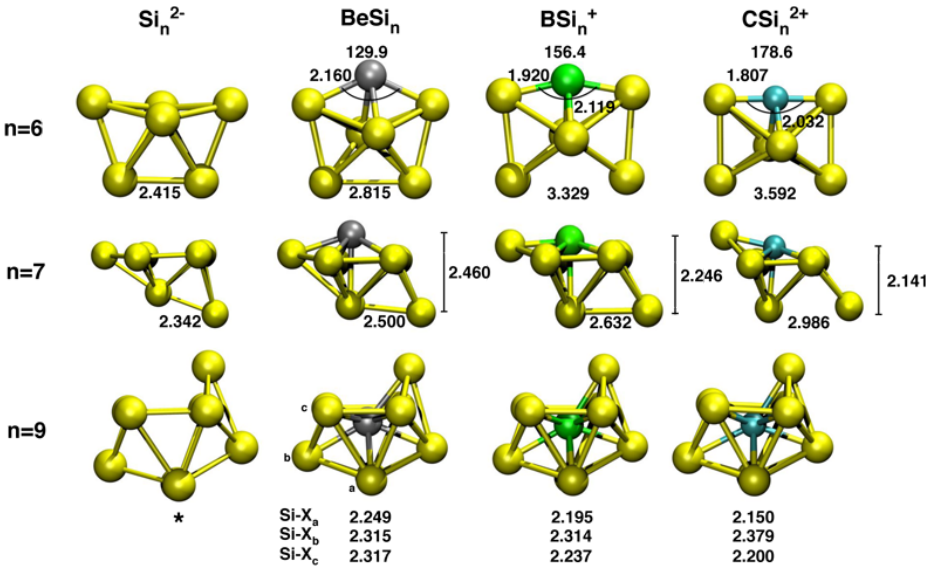

Figure S8: Comparison of the bond distances [Å] in open structures XSi_6, XSi_7 and XSi_9 and Si_n^{2-} bare dianions. The star indicates that the structure is not a stationary point on the PES.

Cartesian coordinates of the XSi_n structures.

$BeSi_6$

7
SCF Done: -1751.82505968
Be 0.890366 0.420885 0.498698
Si -1.165544 0.419764 -0.164981
Si 0.739832 -0.530639 -1.508265
Si -1.357703 -1.782470 -1.259242
Si 0.002483 -1.601906 0.776817
Si 1.218565 -2.869845 -0.938096
Si 2.417474 -1.092361 0.282695
7
SCF Done: -1751.81001965
Be 0.083011 -0.109351 -0.940499
Si -1.340287 -0.939009 0.832179
Si -2.128988 0.008572 -1.114525
Si 0.125113 -2.254793 -0.363907
Si 1.886817 -1.547712 -1.670160
Si 0.435712 -0.475458 -3.103393
Si -0.949648 1.299889 -2.614831
7
SCF Done: -1751.80516600
Be -1.867053 -0.590805 -0.238098
Si -0.926019 1.135345 0.816995
Si -1.574239 -2.608459 0.668511
Si -2.157349 1.427027 -1.145734
Si -1.948824 -0.488291 -2.465502
Si -2.805866 -2.317820 -1.294200
Si -1.782452 -0.693801 1.989361

$BeSi_6$ triplet

7
SCF Done: -1751.79370613
Be 0.291477 0.335521 -2.094314
Si 2.057964 -0.899635 -1.025077
Si -0.472803 -0.912632 0.295773
Si -1.996790 -0.408579 -2.065020
Si -1.171521 1.325180 -0.743624
Si 1.117026 1.048176 -0.155983
Si 0.000446 -1.804373 -1.972180

BSi_6^+

7
SCF Done: -1761.63996689
B -0.730211 1.002880 0.226842
Si -1.703047 -0.869470 0.419427
Si 0.773492 -0.069037 0.753763
Si -0.298614 0.088096 -1.635163
Si 0.187383 -2.076287 -0.581403
Si -2.362140 1.410254 -0.699817
Si -2.588881 -0.766091 -1.869052
7
SCF Done: -1761.63513716
B 0.205989 0.605408 -0.934568
Si 1.457805 1.501602 -2.442745

Si -1.718279 -0.070110 -1.630388
Si -0.805338 1.957604 -2.273316
Si 2.129665 1.282184 -0.238451
Si 1.217672 -0.745765 0.405042
Si -1.045653 -0.289881 0.573745
7
SCF Done: -1761.63377689
B 0.329723 -0.134873 0.832450
Si 1.497184 1.145758 -0.203042
Si 0.584681 -1.918271 -0.040476
Si -1.771229 -0.658869 0.715936
Si -0.052487 -1.300275 2.435083
Si -0.500925 -0.036317 -1.168320
Si -0.747104 1.530701 1.106528

BSi_6^+ triplet
7
SCF Done: -1761.61734080
B 0.674208 -0.851529 -0.908867
Si -1.396885 -0.610737 -1.105750
Si 1.787126 0.432611 0.254976
Si -0.018734 1.366809 -1.302963
Si -0.171488 -0.689846 0.984870
Si 0.125029 -1.285279 -2.868187
Si 1.974300 0.054037 -2.224684

CSi_6^{2+}

7
SCF Done: -1774.45031766
C 2.653962 1.704959 -0.185064
Si 1.139563 2.448126 0.600715
Si -0.588987 1.070376 -1.160270
Si 0.536668 -0.477718 -2.930745
Si 4.410849 1.820822 0.069722
Si -1.871600 -0.114012 -2.660562
Si 1.682109 0.770288 -1.365227
7
SCF Done: -1774.45019070
C 1.133221 0.776392 0.202879
Si 2.345874 1.955599 1.178288
Si -0.885477 0.485901 -0.295488
Si -0.112685 1.438187 1.751750
Si 0.520505 2.446673 -0.669492
Si 0.824652 -0.787879 1.374328
Si 1.289019 -0.533409 -1.230819
7
SCF Done: -1774.44945414
C 0.658003 0.017528 -0.235589
Si 1.033472 -0.879700 1.287095
Si 0.258362 0.942595 -1.735277
Si -1.107458 2.648883 -0.343194
Si 0.964430 1.771072 0.743201
Si -0.336021 0.838057 2.661241
Si -1.252578 0.271348 0.407424
7
SCF Done: -1774.42798473
C -1.866458 -0.590889 -0.238250
Si -0.797297 0.977836 0.695083
Si -1.398547 -2.494341 0.557356

Si -2.333200 1.313147 -1.034603
Si -1.746026 -0.528006 -2.349390
Si -2.934748 -2.160489 -1.172336
Si -1.985525 -0.654063 1.873474

CSi_6^{2+} triplet
7
SCF Done: -1774.42997287
C -0.488859 -1.198892 1.076174
Si -1.066543 0.747702 1.265869
Si -1.689564 -2.531344 1.622859
Si -2.512320 -0.694893 0.046462
Si 1.295548 -0.724294 1.330243
Si -0.341588 -0.804875 -0.919801
Si 0.884104 1.226396 -0.191601

$BeSi_7$
8
SCF Done: -2041.34840318
Be -0.046407 1.009481 2.228010
Si -0.992459 0.489559 0.017207
Si -1.924639 -0.092403 2.343231
Si 0.278216 2.717670 0.892440
Si 0.268478 -1.064493 1.633380
Si -1.997350 2.195018 1.718524
Si 1.554406 0.620260 0.567357
Si -1.802239 -1.792426 0.640031
8
SCF Done: -2041.34704712
Be 1.419704 -0.547958 -0.396520
Si -0.185051 0.973704 -0.104273
Si 0.687800 -2.351360 -1.571955
Si -0.153752 -0.084608 -2.346733
Si 1.834577 1.984082 0.472286
Si -0.650911 -1.328979 0.157580
Si 1.880647 1.188539 -1.718312
Si 2.535774 -0.997252 -2.334792

$BeSi_7$ triplet
8
SCF Done: -2041.31882792
Be 0.030869 -1.345215 -0.012386
Si 0.537319 -1.473689 2.180250
Si 2.876646 -1.053537 -1.007884
Si 1.840948 -2.646058 0.534594
Si 0.647450 0.088519 -1.586295
Si 2.140165 -0.938881 -3.249222
Si 1.632651 0.114129 0.744613
Si 0.838416 -2.417065 -1.776717
BSi_7^+
8
SCF Done: -2051.17880805
B -0.322969 -0.000959 0.678676
Si 0.609057 0.283872 -1.344657
Si -1.414918 1.505462 -0.177171
Si 1.794683 -0.468096 0.943201
Si 0.854679 1.661369 0.889602
Si -0.046457 -1.993568 0.381773
Si -1.810979 -0.715781 -0.751780
Si 0.317967 2.889052 -1.106849

8
SCF Done: -2051.17206617
B -0.072837 0.755324 0.137764
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Si 0.270057 0.486646 -1.923972
Si 1.811432 1.620750 -0.448680
Si -1.367289 1.670261 1.530740
Si -0.384262 2.937064 -0.376959
Si 0.982681 1.471442 1.815768
Si -2.270287 -0.404977 0.863292

BSi_7^+ triplet
8
SCF Done: -2051.14350305
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Si -1.976078 0.463106 0.693130
Si 0.738943 -2.051243 -0.174690
Si 0.509399 0.115383 1.292779
Si -0.146480 -1.191855 -2.302016
Si -1.280911 -0.115263 3.030626
Si -1.131181 -1.897670 1.376074
Si -2.078209 -1.657658 -0.852974

CSi_7^{2+}
8
SCF Done: -2063.98839480
C 0.350679 -0.491053 0.061289
Si 1.984667 -0.603249 -0.844654
Si -2.448345 0.984305 -1.486487
Si -0.083181 0.454126 -1.908221
Si -0.731077 1.154366 0.425339
Si -0.468692 -0.969217 1.805198
Si -1.428239 -1.184537 -0.543165
Si -2.829587 0.010969 1.138323
8
SCF Done: -2063.98676882
C 0.133788 -0.402555 0.043511
Si 1.283529 -1.941703 2.929654
Si -1.211991 -0.967758 1.609985
Si -0.567471 1.487496 1.003287
Si 1.210587 0.094124 1.636207
Si -1.062779 -2.123397 -0.726002
Si -1.170459 0.336997 -1.127192
Si 0.900700 -2.161030 0.557451

CSi_7^{2+} triplet
8
SCF Done: -2063.96434798
C -1.199162 -0.514510 2.355730
Si -1.480223 -1.828219 3.511716
Si -0.143888 -0.467207 0.886753
Si 1.747512 1.013494 0.058533
Si -0.433719 1.888347 -0.110427
Si -1.797749 1.217584 2.150928
Si -0.490982 0.045530 -1.577555
Si 1.377711 -1.275417 -0.717772

$BeSi_8$

9
SCF Done: -2330.86139606
Be -0.401994 -0.360378 -0.672894
Si 1.997407 -0.230768 -0.102973
Si -1.918577 0.912453 0.547563
Si 0.252287 0.404295 1.315761
Si -1.819352 -1.619228 0.916910
Si -2.663693 -0.639008 -1.220465
Si -1.124729 -2.407150 -1.449675
Si 0.817615 -2.168117 0.176749
Si -0.823313 -3.792177 0.606942
9
SCF Done: -2330.85742002
Be -0.962615 0.095848 0.968572
Si -2.623514 -0.840807 2.239567
Si 0.267877 1.621311 1.994650
Si -1.114846 3.639103 1.937575
Si -0.949600 0.205289 -1.320288
Si -2.125534 -1.529529 -0.055933
Si -2.333048 1.540203 2.160988
Si -1.318170 2.174917 0.000368
Si -3.341051 0.693430 0.026075
9
SCF Done: -2330.85562080
Be 1.192291 1.072370 0.262525
Si -0.891566 0.071895 0.125248
Si -0.088221 1.249040 1.996879
Si 0.175361 1.303392 -1.834436
Si -0.955216 -0.931762 -2.112364
Si 1.317691 -0.369488 -3.182915
Si 1.214404 -0.996157 -0.833675
Si 2.592691 0.941481 -1.492524
Si -2.155594 0.356462 2.091376
9
SCF Done: -2330.85556918
Be -0.720691 0.836527 -1.349727
Si -1.021342 -1.145674 1.833445
Si 0.324360 -0.861695 -0.256810
Si -2.364635 2.339307 -0.583311
Si -2.224871 -0.522551 -0.225860
Si 1.230343 0.283368 1.793613
Si 1.248077 1.448479 -0.354312
Si -2.877576 0.686141 -2.141704
Si -0.821291 1.221809 0.984472
9
SCF Done: -2330.85532725
Be -0.484615 -0.119005 0.404490
Si -1.211403 0.375694 -1.832117
Si -1.179105 2.165793 -0.128307
Si 0.740528 1.496447 1.222197
Si 0.370249 -0.656143 2.382658
Si 0.332020 1.470702 3.634748
Si -1.540301 1.206257 2.186848
Si -2.528713 -0.506374 -0.247637
Si -2.020062 -1.226399 2.008309
9
SCF Done: -2330.85511281
Be 1.170819 0.345245 -0.605300
Si 0.987943 0.256434 1.549630
Si 1.325803 2.341635 0.214365

Si 1.017145 -1.651970 -1.424945
Si -0.417186 1.580117 -1.405196
Si -0.746894 -0.508028 -0.076224
Si 2.753988 -0.888387 0.202034
Si 1.342434 0.434443 -2.760254
Si 3.087012 1.196264 -1.139179

$BeSi_8$ triplet

9
SCF Done: -2330.84580505
Be -0.570749 0.663235 0.693004
Si -2.628420 -0.394471 0.914355
Si 1.236298 -0.740487 0.872109
Si 1.516929 1.621643 0.347633
Si -1.969093 0.765357 -1.123747
Si -0.807864 -1.533314 -0.348321
Si 0.470135 0.299898 -1.487428
Si -0.472144 2.619172 -0.540113
Si -0.757214 -1.014168 2.276066

BSi_8^+

9
SCF Done: -2340.70933880
B -0.459238 0.814914 0.491381
Si -0.233902 2.896732 0.094772
Si 1.445125 -0.028996 0.943108
Si 0.848298 1.084080 -1.169781
Si -2.363907 1.662067 0.043055
Si -1.764926 0.549009 2.156470
Si 0.362348 1.783657 2.205431
Si -0.681923 -1.266728 0.895963
Si -1.279944 -0.152472 -1.220012
9
SCF Done: -2340.69081127
B 0.154464 -0.504013 -0.085397
Si 2.826827 -2.223138 -1.581350
Si -0.994124 -2.561507 0.232730
Si -1.706151 -0.204423 0.853651
Si 1.980472 0.054942 -0.904153
Si 1.495833 -2.191211 0.440507
Si 0.353495 -0.775138 2.027472
Si 0.428725 -1.933061 -1.759237
Si -1.389242 -0.357239 -1.559248
9
SCF Done: -2340.68360431
B 1.785774 -0.741745 -1.258754
Si 3.724013 -0.125024 -1.307578
Si 3.121876 -1.751902 0.182530
Si 1.595842 -0.013645 1.006175
Si 0.054413 -1.332997 -0.299298
Si 2.074618 0.632539 -2.959383
Si 0.322975 -1.042071 -2.771186
Si 0.442686 1.041479 -1.103682
Si -1.625204 -0.060976 -1.678521
9
SCF Done: -2340.68198496
B 0.605830 -0.630285 0.828409

Si 0.356647 1.449882 1.216079
Si -1.397471 -0.214670 0.112587
Si -0.607604 -0.434375 2.565283
Si 0.567253 -1.208318 -1.147695
Si 2.351173 0.178291 0.264001
Si -2.563918 -1.623491 1.723591
Si -0.445699 -2.494138 0.805542
Si 1.810633 -1.014988 2.460249
9
SCF Done: -2340.68157168
B -0.298301 0.775462 0.019837
Si -0.232702 0.342607 -2.071417
Si -0.875728 -1.419017 -0.312160
Si 1.512479 -0.325276 -0.255059
Si 1.281950 2.150113 -0.912253
Si 0.837146 1.827375 1.484063
Si -0.275779 -0.423086 1.824029
Si -2.397980 0.509379 -0.230369
Si -1.103231 2.611796 -0.800413
9
SCF Done: -2340.68154958
B -1.387724 -1.020586 1.937240
Si 0.593155 -2.119780 -0.816678
Si 0.142134 -2.524258 1.871231
Si -1.604563 -2.218421 -0.023099
Si 0.330449 -0.272467 0.592720
Si 0.388309 -0.090576 2.904675
Si -2.476902 -2.959980 1.994184
Si -1.724105 0.980152 2.235097
Si -3.398834 -0.697228 1.702785

BSi_8^+ triplet

9
SCF Done: -2340.67068211
B 0.009838 1.286134 0.415300
Si -0.251064 2.012779 -1.469558
Si 1.930203 1.965795 -0.058836
Si -1.257683 -0.488177 -0.263743
Si -2.082542 1.849037 0.080947
Si 1.049802 -0.239889 -1.005078
Si 1.948327 1.516602 -2.472163
Si -1.031035 0.488733 2.026783
Si 1.432593 0.168038 1.497421

CSi_8^{2+}

9
SCF Done: -2353.53141822
C -2.901435 -0.934556 0.970480
Si -2.197653 -0.413477 -0.613096
Si -0.063958 -0.561636 -1.680432
Si -0.340126 1.070128 0.147569
Si -2.103903 1.431214 -1.984441
Si 0.233211 2.000562 -1.830405
Si -0.385002 0.580676 -3.771411
Si -1.955449 0.160802 2.143344
Si -4.163406 -2.112156 1.340094
9
SCF Done: -2353.52760340

C 2.342224 2.450098 0.242260
Si 0.090019 -0.784442 -0.686721
Si 0.937783 3.543670 0.662553
Si -0.030304 1.103703 -2.629945
Si -1.072296 1.712804 -0.345093
Si -1.185434 -0.079186 1.235056
Si 1.277461 1.230674 -0.595180
Si 4.088767 2.533367 0.477171
Si -1.980458 -0.012204 -1.820301
9
SCF Done: -2353.52591537
C -1.717535 1.706110 -0.845671
Si 1.564860 1.866279 1.436988
Si 2.603065 -0.315064 1.878306
Si -3.232340 1.838122 0.065188
Si 1.812738 -0.046694 -0.380952
Si -1.431347 2.176568 -2.530502
Si 0.195941 -0.340599 1.966765
Si -0.227879 1.015492 0.095527
Si 0.465580 -1.941385 0.203033
9
SCF Done: -2353.52438327
C 1.048054 -2.105385 0.299615
Si 2.489094 1.139064 -1.886803
Si 0.315395 2.785599 -1.134775
Si -0.289150 -0.845868 0.361530
Si 0.956119 1.304794 0.584422
Si 1.299232 -3.779004 0.783922
Si 0.207003 0.429502 -1.862369
Si 2.035214 -0.719334 -0.395184
Si -1.710296 0.911563 -0.519287
9
SCF Done: -2353.52392269
C 0.874586 -3.137698 0.907325
Si 1.562314 -4.727490 0.598678
Si -1.219982 2.138061 1.975909
Si 1.822391 0.601154 0.590101
Si -0.825380 -2.493671 0.699213
Si 1.249098 1.874738 2.472601
Si 1.604492 -1.591294 1.534379
Si -0.406810 -0.003297 1.532703
Si 1.150555 -0.246143 3.465792
9
SCF Done: -2353.51678490
C -1.194396 0.333235 0.562815
Si -0.179557 1.649887 -0.760460
Si -0.520422 2.036831 1.637737
Si -1.870041 -1.369783 -0.512868
Si 0.136760 -0.280379 2.101417
Si 0.470430 -0.669082 -0.296918
Si -2.520718 0.949582 -0.977208
Si -2.202660 -0.986359 1.887105
Si -2.860333 1.331327 1.422759

CSi_8^{2+} triplet

9
SCF Done: -2353.51187533
C -0.551627 1.413557 0.454224
Si -1.058149 -2.580205 0.201699

Si 1.242753 -2.091727 0.997439
Si -0.460318 -1.682272 -2.035215
Si -1.550308 2.342896 -0.676217
Si 1.873223 -1.306093 -1.273270
Si -0.048309 -0.346779 -0.064162
Si 0.014899 1.997405 2.028038
Si 0.873666 -3.571339 -1.017362

$BeSi_9$
10
SCF Done: -2620.40348147
Be -0.622895 1.054124 0.610497
Si -0.096634 -1.172080 0.981016
Si -2.399244 -0.333350 0.081868
Si 0.434935 2.878243 1.393749
Si -0.259304 -0.060688 -1.388381
Si -1.897383 0.406964 2.347711
Si 0.495912 0.772646 2.617700
Si 0.246392 2.470888 -1.000674
Si -2.117277 1.903709 -0.840789
Si 1.636063 0.663442 0.271174
10
SCF Done: -2620.40128072
Be -0.250538 0.383262 0.321850
Si -0.970675 -0.392343 -2.520005
Si 0.914354 0.767352 -3.398026
Si 0.036386 -2.503683 -1.619456
Si 0.377625 1.734528 -1.299206
Si -2.036668 1.083543 -0.996667
Si -1.633665 -1.255899 -0.193490
Si 1.747706 -0.675146 -1.697246
Si 0.851728 -1.513244 0.557801
Si 2.058548 0.660243 0.240526

$BeSi_9$ triplet
10
SCF Done: -2620.37040772
Be 0.792799 -0.413309 -0.807831
Si -1.118992 -0.152177 -2.062877
Si -0.143163 -2.338644 -2.172349
Si 1.832934 -0.868006 -2.821301
Si -0.543899 -1.907773 0.196306
Si 0.922483 1.291447 -2.319965
Si 1.872717 -2.241952 -0.209197
Si 1.432604 1.645344 0.022492
Si -0.902371 0.554038 0.254612
Si 2.998296 -0.052270 -0.834620

BSi_9^+
10
SCF Done: -2630.22845883
B 0.362336 0.781628 0.040318
Si -0.933470 -0.318955 1.610131
Si 0.022135 1.248292 -2.121050
Si 1.811132 -0.418318 -1.308194
Si 2.184260 1.853836 -0.550039
Si -0.077055 1.935483 1.854793
Si 0.096353 3.057068 -0.287303
Si 1.335766 -0.928044 1.013573
Si -1.798366 1.314118 -0.185883

Si -0.661083 -0.990926 -0.862356
10
SCF Done: -2630.22500986
B 0.249520 -0.948998 0.176013
Si -0.448557 -2.653292 -0.732847
Si -1.943902 -0.489478 -0.678519
Si -1.908515 1.568791 0.589944
Si 0.720651 -2.071881 1.829945
Si 0.039060 -0.627340 -2.016173
Si 0.336819 1.136175 -0.337089
Si -1.778411 -1.972018 1.334078
Si -0.673893 0.141943 2.102292
Si 1.645029 0.169961 1.500512

BSi_9^+ triplet
10
SCF Done: -2630.20061561
B -0.620319 0.608573 0.235290
Si 1.393975 -0.288373 0.312860
Si -0.665430 -0.394542 2.278875
Si 0.657923 1.553758 1.713972
Si -2.514236 0.985866 1.412366
Si -0.271701 -2.062398 0.609257
Si -1.937154 1.248651 -1.397557
Si -0.026956 -0.295122 -1.647981
Si -2.338406 -0.811938 -0.142920
Si -1.148941 2.723434 0.395637

CSi_9^{2+}
10
SCF Done: -2643.07457409
C -1.874316 -1.795571 -0.326140
Si 0.210709 1.452188 0.599499
Si -0.327439 3.373652 -1.030853
Si 0.163984 1.095016 -2.126694
Si -0.518271 -0.583143 -0.508006
Si -1.790643 -3.537452 -0.097957
Si -1.897316 1.545365 -0.763282
Si 2.028749 2.135428 -0.908199
Si 1.852585 -0.317872 -0.584543
Si -3.390296 -0.754542 -0.440689
10
SCF Done: -2643.05940218
C -0.332006 1.761196 -0.718117
Si -0.046162 0.188975 0.134797
Si 0.240644 1.270871 -2.407703
Si -0.855774 -2.033289 0.223928
Si 1.711124 -1.222012 0.858985
Si 0.616057 -3.216970 1.809582
Si 0.847419 -1.214224 -1.678999
Si 1.229705 -3.362494 -0.484330
Si 1.723104 -3.108342 -2.785511
Si -0.946027 3.337993 -0.248517
10
SCF Done: -2643.02177847
C 0.340513 0.776693 0.019638
Si -0.980947 -0.352467 1.644504
Si 0.040021 1.253272 -2.107605
Si 1.841030 -0.454410 -1.356692
Si 2.148245 1.820495 -0.497025

Si -0.028278 1.899218 1.816460
Si 0.078072 3.119051 -0.306896
Si 1.331600 -0.856530 1.006992
Si -1.783726 1.319032 -0.168962
Si -0.644524 -0.990171 -0.846424

CSi_9^{2+} triplet
10
SCF Done: -2643.02983565
C -1.974481 -1.311630 3.006749
Si 1.585346 1.463720 0.063198
Si -0.401900 -1.163646 2.043357
Si 0.035751 1.319858 1.915697
Si -0.114033 1.286513 -2.129152
Si -0.279814 -0.068633 -0.257817
Si -2.037272 0.430464 3.492976
Si -1.110153 2.301941 0.086591
Si -3.030306 -2.627137 3.511753
Si 0.679825 3.362870 -1.127665

$BeSi_{10}$
11
SCF Done: -2909.94622090
Be -0.074146 -0.847716 0.340139
Si 0.448033 -2.371162 -1.213698
Si 0.357792 -0.375869 2.485629
Si 2.039175 -1.330653 0.897902
Si -0.802153 0.161826 -1.519882
Si -1.888656 -1.536907 2.048577
Si 0.789472 1.202241 0.592138
Si 0.116338 -2.902037 1.208993
Si -1.651034 0.680089 0.776487
Si -1.892498 -1.845982 -0.499649
Si 1.740317 -0.157908 -1.365459
11
SCF Done: -2909.93459701
Be -0.554953 1.435134 -0.400615
Si -0.616142 -1.428901 3.288955
Si -1.030967 -1.883377 0.955946
Si -0.108022 2.286950 1.582863
Si -1.740610 0.384366 2.223078
Si 1.673363 1.229309 0.145118
Si 0.790063 -0.122329 1.872466
Si -1.054786 0.227546 -2.264070
Si 0.336915 -0.789512 -0.672305
Si -2.258319 -0.270146 -0.312384
Si -2.467238 2.059207 0.720326

$BeSi_{10}$ triplet
11
SCF Done: -2909.92204260
Be -0.024343 -0.527881 0.127197
Si -2.267141 -1.135047 -0.109813
Si -0.610631 -2.297016 1.298511
Si 0.818629 1.567740 0.468555
Si 1.444613 0.035428 -1.529601
Si -0.964520 0.971651 -1.318469
Si -1.569613 0.875150 1.202347
Si 2.201376 -0.588554 0.871272
Si 1.160188 -2.467315 -0.407940

Si -0.590011 -1.522447 -1.923224
Si 0.269033 -0.291680 2.430445

BSi_{10}^{+}
11
SCF Done: -2919.77151569
B -0.913609 -0.362704 0.125791
Si -0.589466 -0.086646 -2.001032
Si 1.650515 -0.008223 1.604811
Si -0.238370 -1.764855 1.756389
Si -1.158368 -2.441701 -0.442059
Si -0.750564 0.853361 2.017012
Si 1.028723 -1.283416 -0.555645
Si 0.514719 1.331992 -0.294533
Si -1.942253 1.538859 -0.044929
Si -2.513504 -0.814260 1.518649
Si -2.885083 -0.639094 -1.007803
11
SCF Done: -2919.76673124
B 0.851312 -0.286917 -0.446180
Si -0.616659 -1.509984 1.249340
Si 0.935084 0.730559 1.274270
Si -0.113995 -0.105180 -2.257671
Si 0.622698 -2.252457 -1.023181
Si -0.720375 -2.317165 -3.038858
Si -1.419225 0.827271 -0.094826
Si 1.779441 -1.668618 0.969290
Si 0.586078 1.803188 -1.026208
Si -2.874087 -0.770266 0.938708
Si -1.895979 -1.578543 -1.048556

BSi_{10}^{+} triplet
11
SCF Done: -2919.73867175
B -0.265064 0.296751 -0.235033
Si -1.219402 2.414446 -0.765971
Si -1.912285 -0.984377 -0.849703
Si 1.687181 -0.072832 0.839981
Si -2.363004 0.826052 0.763722
Si -0.649897 -0.743025 1.714555
Si 0.040467 1.735026 1.481256
Si -0.804040 0.550500 -2.329036
Si 1.385816 -0.446788 -1.780843
Si 1.231277 1.864093 -0.807492
Si 0.239024 -2.030801 -0.248918

CSi_{10}^{2+}
11
SCF Done: -2932.60038476
C 3.507394 -0.517092 0.554543
Si 0.134007 -0.647629 0.933555
Si 5.254453 -0.402099 0.435159
Si -1.931933 0.937110 -2.136201
Si -1.162193 1.315144 0.249494
Si -3.428679 0.449350 -0.069151
Si -2.097694 -0.570567 1.838270
Si 2.480507 0.294363 1.784007
Si -1.676316 -1.166445 -0.672788
Si 0.285944 0.131439 -1.470029
Si 2.141756 -1.490187 -0.267699

11
SCF Done: -2932.59931123
C -0.753174 -0.328511 1.007556
Si 2.344185 1.644771 1.279037
Si -1.120831 0.847633 -0.960286
Si -0.098487 -1.511138 -0.340532
Si -0.039867 1.878500 1.131671
Si 2.040398 0.015816 -0.602217
Si 0.990992 -0.471849 1.770844
Si 0.401818 -0.207204 -2.486981
Si -2.253958 0.749475 1.252385
Si 2.084147 -2.185023 0.456897
Si 1.041622 2.209619 -1.168424
11
SCF Done: -2932.56980495
C -0.984189 -0.373109 0.085526
Si -0.597691 -0.088974 -1.989269
Si 1.711719 0.000470 1.638971
Si -0.225903 -1.753078 1.755671
Si -1.162835 -2.428455 -0.441197
Si -0.734481 0.847563 2.014903
Si 1.033142 -1.275283 -0.541216
Si 0.522623 1.323942 -0.282164
Si -1.941058 1.524453 -0.046829
Si -2.508775 -0.811686 1.505272
Si -2.909811 -0.642530 -1.023018

CSi_{10}^{2+} triplet
11
SCF Done: -2932.56812218
C 1.572433 2.269945 -0.320138
Si 0.783296 2.697798 1.471582
Si -0.656793 -0.911150 -0.392577
Si -1.524009 2.633556 0.804379
Si 1.347405 -1.058411 0.868482
Si -0.161184 1.439321 -0.781320
Si 2.612876 0.948139 0.655923
Si 2.377090 3.497238 -1.320586
Si 2.595588 1.901969 2.863093
Si 1.054286 0.034764 2.943065
Si -0.949652 0.419272 1.575705

Si_6 GM
6
SCF Done: -1737.06650869
Si -0.765755 1.682022 1.474371
Si 0.645012 -0.260519 1.112312
Si 0.876565 2.057515 -0.273796
Si -0.539929 0.259450 -0.867211
Si 1.644540 1.762419 2.010853
Si 2.543898 0.379195 -0.150532

Si_6^{2-} GM
6
SCF Done: -1737.08330801
Si 1.002978 -1.215700 -0.085901
Si 0.624202 0.262795 -2.056590
Si 0.455988 2.236109 -0.543241
Si 2.467389 0.767074 -0.456432
Si 0.834872 0.757472 1.427199

Si -1.008423 0.253390 -0.173240

Si_6^{2-} open structure
6
SCF Done: -1737.06699697
Si 1.792688 1.452691 0.560564
Si 0.532491 3.415928 -0.003161
Si 0.018235 -0.128385 1.725089
Si -0.791546 1.352943 -0.002186
Si 0.204879 2.472373 2.179091
Si 1.893160 0.926625 2.900187

Si_6^{2-} D_{3d} ring
6
SCF Done: -1737.01240572
Si -0.876362 1.039108 0.746032
Si -1.494311 -2.529092 0.604402
Si -2.237219 1.348322 -1.081886
Si -1.851427 -0.508456 -2.382871
Si -2.855574 -2.222232 -1.223611
Si -1.879856 -0.673649 1.907364

Si_7 GM
7
SCF Done: -2026.60167543
Si 0.230366 -0.469492 0.373752
Si -0.099693 0.946499 2.396634
Si -0.229496 1.964017 0.107010
Si 1.480143 0.834834 -1.341329
Si 1.689615 -0.811714 2.363538
Si 1.972274 1.290454 1.057190
Si 2.666076 -0.880829 0.053307

Si_7^{2-} GM
7
SCF Done: -2026.60575600
Si -1.523324 -0.532495 0.284615
Si 1.241025 -1.370473 -2.310958
Si -0.130140 -2.251815 1.213898
Si -0.676016 0.011913 -1.893760
Si 1.080126 -0.223403 0.052493
Si 1.578159 -2.769846 -0.390358
Si -0.884324 -2.541429 -1.291034

Si_7^{2-} open structure
7
SCF Done: -2026.57397550
Si 0.438140 0.303867 -0.985103
Si -1.415131 1.616822 -0.002349
Si 1.759886 -0.448701 0.962399
Si 0.707185 1.762554 0.995775
Si 0.140331 -1.985255 -0.015985
Si -1.806158 -0.694046 -0.713153
Si 0.479780 2.607069 -1.407466

Si_8 GM
8
SCF Done: -2316.09454434
Si -0.418259 -2.939313 -0.143953
Si -1.144739 -0.866919 -1.303483

Si 1.638361 -2.306578 0.963937
Si 1.442310 -0.017707 2.017851
Si -0.614394 -0.650461 0.910063
Si -0.248385 -2.296804 2.646164
Si 1.272379 -0.660266 -0.772169
Si 2.168762 -2.090101 3.177449

Si_8^{2-} GM
8
SCF Done: -2316.15315994
Si 0.434826 -1.643458 -0.814367
Si 0.628742 0.601715 -1.708370
Si -0.113997 2.095247 0.050779
Si 0.435271 -0.057983 1.019678
Si 2.695281 -0.842346 -0.460495
Si 2.297186 1.871293 0.167501
Si 3.001059 1.014778 -1.988663
Si 2.734388 0.105699 1.770497

Si_8^{2-} O_h cubic cage
8
SCF Done: -2316.11836965
Si -0.240721 2.841858 0.104840
Si 1.395135 -0.007235 0.930925
Si 0.813985 1.076611 -1.125718
Si -2.313706 1.639868 0.055084
Si -1.730729 0.556060 2.111417
Si 0.341296 1.758658 2.161109
Si -0.676213 -1.211596 0.884070
Si -1.257877 -0.126875 -1.172720

Si_9 GM
9
SCF Done: -2605.62989214
Si -0.761539 -0.312153 -1.333548
Si -0.130745 3.533524 -1.192358
Si 0.600100 1.500802 -2.326411
Si 1.393918 -0.030399 0.112982
Si -0.699467 1.700611 0.220977
Si 1.714103 2.668403 0.043004
Si 0.933308 1.454791 1.938178
Si 1.530577 -0.780602 -2.122780
Si 2.946061 1.173985 -1.606059

Si_9^{2-} GM
9
SCF Done: -2605.68500237
Si -0.031975 0.189541 1.565696
Si -1.127316 -1.807580 2.944803
Si -0.972794 -1.949927 0.291367
Si -1.469287 0.569924 3.545591
Si -1.229290 0.347251 -0.596076
Si -2.368254 1.335172 1.368460
Si -3.309905 -0.804350 0.093956
Si -2.938444 -2.768045 1.556140
Si -3.464081 -0.661334 2.747211

Si_{10} GM
10
SCF Done: -2895.17393335

Si	-1.357914	-0.498061	0.837318
Si	0.681105	-2.007283	1.204828
Si	1.936039	1.138266	-1.780355
Si	0.013941	1.215031	-0.416606
Si	0.615711	-0.759731	-2.246514
Si	1.693282	-2.610272	-1.015714
Si	0.768977	0.432316	1.800226
Si	-1.684472	-0.109497	-1.624810
Si	-0.799633	-2.333665	-0.861398
Si	2.208410	-0.409263	-0.021942

Si_{10} D_{4d}
10
SCF Done: -2895.14261999

Si	-1.124416	-0.913938	-1.429515
Si	1.814570	0.088579	1.379458
Si	2.544843	-0.724334	-0.744054
Si	0.551027	2.068984	0.737500
Si	2.183802	1.620082	-1.013406
Si	0.997560	-0.490864	-2.547340
Si	0.628838	-2.021050	-0.152074
Si	-1.426961	1.103415	-0.187937
Si	-0.024893	1.659964	-2.038458
Si	-0.548293	-0.503060	1.345531

Si_{10}^{2-} GM
10
SCF Done: -2895.23465641

Si	-0.617458	-0.103660	-1.871073
Si	1.544162	-0.023244	1.541947
Si	-0.223288	-1.772961	1.774450
Si	-1.151280	-2.312081	-0.409638
Si	-0.740030	0.864315	2.037587
Si	1.052606	-1.290030	-0.555974
Si	0.535054	1.346462	-0.291556
Si	-1.885088	1.417291	-0.038447
Si	-2.420875	-0.786829	1.425622
Si	-2.906875	-0.642840	-1.021793