Supporting information

Determination of ionization energies of small silicon clusters with vacuum-ultraviolet (VUV) radiation.

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Atomic coordinates for silicon clusters shown in Figure 2 in neutral and cationic states (XYZ file format in Angstrom)

1. Neutral clusters

Si_2

0.0000000	0.0000000	1.1403090
0.0000000	0.0000000	-1.1403090

Si_3

0.0000000	0.0000000	1.0974400
0.0000000	1.4377490	-0.5487200
0.0000000	-1.4377490	-0.5487200

Si_4

-1.0361450	0.6333590	0.0000000
1.0361450	1.6951430	0.0000000
1.0361450	-0.6333590	0.0000000
-1.0361450	-1.6951430	0.0000000

Si_5

0.0001110	0.0000510	1.4754400
0.0001110	0.0000510	-1.4754400
1.5614660	0.9017510	0.0000000
-1.5618000	0.9014180	0.0000000
0.0001110	-1.8032710	0.0000000

Si_6

0.0002550	-0.1763350	1.3515410
0.0002550	-0.1763350	-1.3515410
1.9498550	0.2944950	0.0000000
-1.9493670	0.2952090	0.0000000
-0.0012520	-2.0889960	0.0000000
0.0002550	1.8519620	0.0000000

Si_7

-1.2548270	1.7272610	0.0000000
1.2549200	1.7270640	0.0000000
2.0304420	-0.6598570	0.0000000
-0.0000540	-2.1349740	0.0000000
-2.0303730	-0.6596580	0.0000000
-0.0000540	0.0000820	1.2875210
-0.0000540	0.0000820	-1.2875210

2. Cationic clusters

Si_2

0.0000000	0.0000000	1.1512950
0.0000000	0.0000000	-1.1512950

Si_3

0.0000000	0.0000000	1.2353690
0.0000000	1.2613020	-0.6176840
0.0000000	-1.2613020	-0.6176840

Si_4

-1.0907970	0.7796020	0.0000000
-1.0907970	-1.5262190	0.0000000
1.0907970	-0.7796020	0.0000000
1.0907970	1.5262190	0.0000000

Si_5

-0.0000410	0.0096130	1.5673300
-0.0000410	0.0096130	-1.5673300
-1.6068600	-0.8329240	0.0000000
1.6069830	-0.8328260	0.0000000
-0.0000410	1.6465260	0.0000000

Si_6

-0.2260650	-0.0710560	1.4282980
-0.2260650	-0.0710560	-1.4282980
0.8552300	-1.6235090	0.0000000
-0.2260650	1.8209810	0.0000000
-2.0452860	-0.6418790	0.0000000
1.8682500	0.5865200	0.0000000

Si_7

1.7977430	-0.7689750	0.0000000
-0.1081530	-2.1935130	0.0000000
-2.0610900	-0.6899310	0.0000000
-0.9239610	1.9674290	0.0000000
1.5117660	1.5929220	0.0000000
-0.1081530	0.0460330	1.3262760
-0.1081530	0.0460330	-1.3262760

Atomic coordinates for tetramer silicon isomers shown in Figure 4 in neutral and cationic states (XYZ file format in Angstrom)

1. **Neutral clusters**

D_{2h}

$^{1}A_{g}$

-1.0931440	0.6867670	0.0000000
-1.0931440	-1.7401850	0.0000000
1.0931440	-0.6867670	0.0000000
1.0931440	1.7401850	0.0000000

$^{3}A_{u}$

-1.1179700	0.7703670	0.0000000
-1.1179700	-1.6224540	0.0000000
1.1179700	-0.7703670	0.0000000
1.1179700	1.6224540	0.0000000

T_{d}

^{1}A

1.2576050	-0.6298330	-0.8279160
0.3134500	1.5603410	0.3612840
-1.3504030	-0.0864570	-0.9125120
-0.2206520	-0.8440510	1.3791440

^{3}A

-0.2076680	-1.5999930	-0.3726930
1.6016190	-0.2073550	0.3725800
0.2072660	1.6001210	-0.3726590
-1.6012170	0.2072270	0.3727720

C_{2v}

$^{3}A''$

1.7419090	-0.9834770	0.0000000
-0.4583420	-1.9679410	0.0000000
0.0000000	0.5292250	0.0000000
-1.2835670	2.4221930	0.0000000

$D_{\infty h}$

^{1}A

3.3432070	-0.0019440	0.0022900
1.1003950	-0.0001930	-0.0000680
-1.1003950	-0.0001350	-0.0008400
-3.3432070	0.0022720	-0.0013830

$^{3}\Sigma_g^-$

0.0000000	0.0000000	3.3482680
0.0000000	0.0000000	1.0969530
0.0000000	0.0000000	-1.0969530
0.0000000	0.0000000	-3.3482680

2. Cationic clusters

D_{2h}

$^{2}B_u$

-1.1463120	0.8348170	0.0000000
1.1463120	1.5740530	0.0000000
1.1463120	-0.8348170	0.0000000
-1.1463120	-1.5740530	0.0000000

C_{2v}

$^{2}A'$

1.3048810	-1.5714160	0.0000000
-1.2990580	-1.5753770	0.0000000
0.0000000	0.4264340	0.0000000
-0.0058230	2.7203590	0.0000000

$^{4}A''$

-1.1608340	-1.6831510	0.0000000
1.1771790	-1.6742780	0.0000000
0.0000000	0.4806730	0.0000000
-0.0163450	2.8767550	0.0000000

$D_{\infty h}$

^{2}A

3.4096490	0.0004250	0.0001720
1.0839710	-0.0003560	-0.0004390
-1.0839710	-0.0005590	0.0003440
-3.4096490	0.0004900	-0.0000770

$^{4}\Sigma_{g}^{-}$

0.0000000	0.0000000	3.4647570
0.0000000	0.0000000	1.1488940
0.0000000	0.0000000	-1.1488940
0.0000000	0.0000000	-3.4647570

Bond lengths for silicon clusters shown in Figure 2 in neutral and cationic states (in Angstroms)

1. Neutral clusters

Si_2

R(1,2)	2.2806

Si_3

R(1,2)	2.1856
R(1,3)	2.1856

Si_4

R(1,2)	2.3285
R(1,3)	2.4288
R(1,4)	2.3285
R(2,3)	2.3285
R(3,4)	2.3285

Si_5

R(1,3)	2.3298
R(1,4)	2.33
R(1,5)	2.33
R(2,3)	2.3298
R(2,4)	2.33
R(2,5)	2.33

Si_6

R(1,2)	2.7031
R(1,3)	2.4185
R(1,4)	2.4187
R(1,5)	2.342
R(1,6)	2.4373

R(2,3)	2.4185
R(2,4)	2.4187
R(2,5)	2.342
R(2,6)	2.4373
R(3,6)	2.4953
R(4,6)	2.4949

Si_7

R(1,2)	2.5097
R(1,5)	2.5098
R(1,6)	2.4931
R(1,7)	2.4931
R(2,3)	2.5097
R(2,6)	2.493
R(2,7)	2.493
R(3,4)	2.5098
R(3,6)	2.4932
R(3,7)	2.4932
R(4,5)	2.5097
R(4,6)	2.4932
R(4,7)	2.4932
R(5,6)	2.493
R(5,7)	2.493
R(6,7)	2.575

2. Cationic clusters

Si_2

R(1,2)	2.3026

Si_3

R(1,2)	2.2416
R(1,3)	2.2416
R(2,3)	2.5226

Si_4

R(1,2)	2.3058
R(1,3)	2.6815
R(1,4)	2.3058
R(2,3)	2.3058
R(3,4)	2.3058

Si_5

R(1,3)	2.3976
R(1,4)	2.3977
R(1,5)	2.2663
R(2,3)	2.3976
R(2,4)	2.3977
R(2,5)	2.2663

Si_6

R(1,2)	2.8566
R(1,3)	2.3705
R(1,4)	2.3706
R(1,5)	2.3823

R(1,6)	2.6189
R(2,3)	2.3705
R(2,4)	2.3706
R(2,5)	2.3823
R(2,6)	2.6189
R(3,6)	2.4311
R(4,6)	2.4311

Si_7

R(1,2)	2.3794
R(1,5)	2.3791
R(1,6)	2.4608
R(1,7)	2.4608
R(2,3)	2.4647
R(2,6)	2.6028
R(2,7)	2.6028
R(3,4)	2.8904
R(3,6)	2.4728
R(3,7)	2.4728
R(4,5)	2.4644
R(4,6)	2.4731
R(4,7)	2.4731
R(5,6)	2.6031
R(5,7)	2.6031
R(6,7)	2.6526

Bond lengths for tetramer silicon isomers shown in Figure 4 in neutral and cationic states (in Angstroms)

1. **Neutral clusters**

D_{2h}

^1A_g

R(1,2)	2.427
R(1,3)	2.5819
R(1,4)	2.4268
R(2,3)	2.4268
R(3,4)	2.427

^3A_u

R(1,2)	2.3928
R(1,3)	2.7154
R(1,4)	2.3928
R(2,3)	2.3928
R(3,4)	2.3928

T_d

^1A

R(1,2)	2.665
R(1,3)	2.6654
R(1,4)	2.665
R(2,3)	2.6651
R(2,4)	2.665
R(3,4)	2.665

^3A

R(1,2)	2.4017
R(1,4)	2.4008
R(2,3)	2.4014
R(3,4)	2.4013

C_{2v}

$^3A''$

R(1,2)	2.4105
R(1,3)	2.3071
R(2,3)	2.5389
R(3,4)	2.2871

$D_{\infty h}$

^1A

R(1,2)	2.2428
R(2,3)	2.2008
R(3,4)	2.2428

$^3\Sigma_g^-$

R(1,2)	2.2513
R(2,3)	2.1939
R(3,4)	2.2513

2. Cationic clusters

D_{2h}

^2B_u

R(1,2)	2.4089
R(1,3)	2.8362
R(1,4)	2.4089
R(2,3)	2.4089
R(3,4)	2.4089

C_{2v}

$^2A'$

R(1,2)	2.6039
R(1,3)	2.3862
R(2,3)	2.3864
R(3,4)	2.2939

$^4A''$

R(1,2)	2.338
R(1,3)	2.4555
R(2,3)	2.4555
R(3,4)	2.3961

$D_{\infty h}$

^2A

R(1,2)	2.3257
R(2,3)	2.1679
R(3,4)	2.3257

$^4\Sigma_g^-$

R(1,2)	2.3159
R(2,3)	2.2978
R(3,4)	2.3159