Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information File

Tip Enhanced Raman Spectroscopy (TERS) as a Probe for the Buckling Distortion in Silicene

Available Information:

1. Cartesian Coordinates for Optimized Structures and their Energies in Hartrees.
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4. Results of calculations done at PBE1PBE/6-311+G(d,p) level of theory.
5. Normal Modes for which Scattering Activity decreases/increases due to coordination to Clusters (at M05-2X/TZVP and PBE1PBE/6-311+G(d,p) levels of theory.)

M05-2X/TZVP

Si_6H_6:

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.000000	3.659946	0.041316
1	3.169606	1.829973	-0.041316
1	3.169606	-1.829973	0.041316
1	0.000000	-3.659946	-0.041316
1	-3.169606	-1.829973	0.041316
1	-3.169606	1.829973	-0.041316
14	-1.898055	-1.095842	-0.196987
14	0.000000	-2.191685	0.196987
14	1.898055	-1.095842	-0.196987
14	1.898055	1.095842	0.196987
14	0.000000	2.191685	-0.196987
14	-1.898055	1.095842	0.196987

M05-2X/TZVP = -1740.4577049 Hartree

Low frequencies (cm^{-1}): 99.4119 99.4167 128.3781 141.4953 142.8202 193.1578 366.6978 394.6685 394.904 396.2289

$Si_{10}H_8$:

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-0.067309	3.668995	1.920033
1	0.020728	1.820375	-5.094686
1	-0.067309	3.668995	-1.920033
1	0.067309	-3.668995	-1.920033
1	-0.020728	-1.820375	-5.094686
1	0.067309	-3.668995	1.920033
1	-0.020728	-1.820375	5.094686
1	0.020728	1.820375	5.094686
14	-0.227334	1.108370	0.000000
14	0.227334	-1.108370	0.000000
14	-0.194045	-2.203051	1.931127
14	0.194045	2.203051	1.931127
14	-0.194045	1.107298	3.806647
14	0.194045	-1.107298	3.806647
14	0.194045	2.203051	-1.931127
14	-0.194045	-2.203051	-1.931127
14	-0.194045	1.107298	-3.806647
14	0.194045	-1.107298	-3.806647

M05-2X/TZVP = -2899.6107718 Hartree

Low frequencies (cm^{-1}): 34.7884 51.8558 72.0719 86.9749 97.9990 103.4098 111.4081 119.7183 122.3147 140.0141

$Si_{14}H_{10}$ (A):

Atomic Number	Coordinates (Angstroms) X	Y	Z

14	-0.194044	2.212745	3.855489
14	-0.220187	2.198940	0.000000
14	-0.194044	2.212745	-3.855489
14	0.194044	1.112129	5.719929
14	0.222341	1.116367	1.912176
14	0.222341	1.116367	-1.912176
14	-0.194044	-1.112129	5.719929
14	-0.222341	-1.116367	1.912176
14	-0.222341	-1.116367	-1.912176
14	0.194044	-2.212745	3.855489
14	0.220187	-2.198940	0.000000
1	-0.073673	-3.677257	3.843129
1	-0.075669	-3.660386	0.000000
14	0.194044	-2.212745	-3.855489
1	-0.073673	-3.677257	-3.843129
14	-0.194044	-1.112129	-5.719929
1	0.004712	-1.815278	-7.015682
14	0.194044	1.112129	-5.719929
1	-0.004712	1.815278	7.015682
1	0.004712	-1.815278	7.015682
1	-0.004712	1.815278	-7.015682
1	0.073673	3.677257	3.843129
1	0.075669	3.660386	0.000000
1	0.073673	3.677257	-3.843129

M05-2X/TZVP = -4058.7606744 Hartree

Low frequencies (cm^{-1}): 13.0982 30.2674 46.7224 51.1724 67.1646 68.9311
85.1635 97.8236 98.9753 101.8837

$Si_{14}H_{10}$ (B):

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.037834	-5.137555	2.649862
1	-0.012941	1.843745	4.540436
1	0.017519	7.001900	-0.514330
1	-0.037834	5.137555	2.649862
1	-0.046789	1.545453	-3.730878
1	-0.112069	5.203975	-3.687861
1	0.012941	-1.843745	4.540436
1	-0.017519	-7.001900	-0.514330
1	0.112069	-5.203975	-3.687861
1	0.046789	-1.545453	-3.730878
14	-0.193331	5.528994	-0.506298
14	0.214924	4.424093	1.367971
14	-0.203392	2.213849	1.356343
14	0.214924	1.076034	3.284968
14	-0.214924	-1.076034	3.284968
14	0.203392	-2.213849	1.356343
14	-0.239141	-1.121365	-0.570210
14	0.239141	1.121365	-0.570210
14	-0.262875	2.264357	-2.444232
14	0.142694	4.442226	-2.435487
14	0.262875	-2.264357	-2.444232
14	-0.142694	-4.442226	-2.435487
14	0.193331	-5.528994	-0.506298
14	-0.214924	-4.424093	1.367971

M05-2X/TZVP = -4058.768055 Hartree

Low frequencies (cm^{-1}): 28.7101 31.5083 48.6043 61.1931 66.5771 92.0058
92.1837 97.5808 99.6525 107.9377

$Si_{18}H_{12}$ (A):

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-6.770070	-2.650606	0.079771
1	-7.203902	0.982743	-0.023604
1	4.452612	5.745416	-0.065521
1	1.087057	7.186428	0.007220
1	2.754473	-6.725043	-0.106109
1	5.680927	-4.536610	0.068358
1	5.244719	-0.896152	0.061732
1	4.886112	2.107975	0.029418
1	-1.844319	4.991407	-0.040567
1	-4.271095	3.176955	0.013289
1	-3.402216	-4.093372	0.002224
1	-0.614539	-5.285441	-0.059677
14	3.533601	2.686159	-0.199421
14	1.779778	1.352987	0.233658
14	-0.249007	2.218534	-0.218578
14	-0.492810	4.411951	0.190957
14	1.252804	5.722592	-0.199045
14	3.281218	4.858421	0.164959
14	2.052469	-0.893546	-0.190705
14	0.277845	-2.220992	0.204629
14	-1.800763	-1.327615	-0.219684
14	-2.061004	0.866028	0.212762
14	-4.096071	1.715318	-0.209080
14	-5.846389	0.412937	0.187533
14	-5.588010	-1.779127	-0.155142
14	-3.575214	-2.630788	0.219984
14	0.564677	-4.398858	-0.258986
14	2.565256	-5.270076	0.138204
14	4.336887	-3.942203	-0.160272
14	4.064751	-1.781984	0.260617

M05-2X/TZVP = -5217.9273411 Hartree

Low frequencies (cm^{-1}): 3.0233 16.5951 26.0587 36.5386 41.7134 42.3524
68.2427 70.1244 90.7684 94.8885.

$Si_{18}H_{12}$ (B):

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-3.674308	-0.072704	1.941712
1	-3.674308	-0.072704	-1.941712
1	-1.785350	-0.218444	-8.932836
1	-3.665717	-0.208543	-5.776262
1	3.689182	0.112984	-5.741684
1	1.839510	-0.114518	-8.927353
1	3.648563	0.200528	-1.907308

1	3.648563	0.200528	1.907308
1	-1.785350	-0.218444	8.932836
1	1.839510	-0.114518	8.927353
1	3.689182	0.112984	5.741684
1	-3.665717	-0.208543	5.776262
14	1.132378	0.118885	-7.639576
14	-1.084863	-0.334845	-7.625678
14	2.230780	-0.184570	-5.761694
14	-2.209209	0.098310	-5.789056
14	1.111213	0.270001	-3.835216
14	-1.119981	-0.213271	-3.817547
14	2.188977	-0.102482	-1.917347
14	-2.224421	0.274456	-1.937285
14	1.089165	0.328657	0.000000
14	-1.146325	-0.138669	0.000000
14	2.188977	-0.102482	1.917347
14	-2.224421	0.274456	1.937285
14	1.111213	0.270001	3.835216
14	-1.119981	-0.213271	3.817547
14	2.230780	-0.184570	5.761694
14	-2.209209	0.098310	5.789056
14	1.132378	0.118885	7.639576
14	-1.084863	-0.334845	7.625678

M05-2X/TZVP = -5217.9092157 Hartree

Low frequencies (cm^{-1}): 8.7912 22.4977 31.4099 33.6787 49.5205 50.7371
67.1805 70.4935 80.0715 86.2443

$Si_{22}H_{14}$:

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	3.727579	-0.061455	0.000000
1	3.680647	0.072843	3.906835
1	1.719025	0.492904	10.838638
1	3.628891	0.370851	7.700741
1	-3.727550	-0.022855	7.623220
1	-1.897974	0.339455	10.816439
1	-3.637632	-0.260522	3.772391
1	-3.596433	-0.360167	0.000000
1	3.680647	0.072843	-3.906835
1	-3.637632	-0.260522	-3.772391
1	3.628891	0.370851	-7.700741
1	-3.727550	-0.022855	-7.623220
1	-1.897974	0.339455	-10.816439
1	1.719025	0.492904	-10.838638
14	-1.131713	-0.254032	5.753133
14	1.098898	0.244736	5.720218
14	2.239163	-0.306472	3.881042
14	1.196187	0.025898	1.902309
14	2.292652	-0.468060	0.000000
14	1.196187	0.025898	-1.902309
14	2.239163	-0.306472	-3.881042
14	1.098898	0.244736	-5.720218
14	2.177419	0.043047	-7.714526
14	1.029409	0.533670	-9.521027
14	-1.185837	0.057487	-9.541163
14	-2.271733	0.287008	-7.646592

14	-1.131713	-0.254032	-5.753133
14	-2.178510	0.042442	-3.809217
14	-1.041937	-0.452546	-1.923670
14	-2.131201	-0.086110	0.000000
14	-1.041937	-0.452546	1.923670
14	-2.178510	0.042442	3.809217
14	-2.271733	0.287008	7.646592
14	2.177419	0.043047	7.714526
14	1.029409	0.533670	9.521027
14	-1.185837	0.057487	9.541163

M05-2X/TZVP = -6377.0571657 Hartree

Low frequencies (cm^{-1}): 10.3810 20.6743 22.3987 23.2645 39.4008 42.0170
45.3463 58.2593 65.0351 69.9632

$Si_{16}H_{10}$:

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.203175	-1.078137	3.852083
14	0.234877	2.216056	1.923529
14	0.156455	5.509955	0.000000
14	-0.203175	1.078137	3.852083
14	-0.234877	-2.216056	1.923529
14	-0.203175	4.411964	1.902681
14	-0.237233	1.112374	0.000000
14	-0.203175	4.411964	-1.902681
14	0.203175	-4.411964	1.902681
14	0.237233	-1.112374	0.000000
14	0.234877	2.216056	-1.923529
14	-0.156455	-5.509955	0.000000
14	-0.234877	-2.216056	-1.923529
14	-0.203175	1.078137	-3.852083
14	0.203175	-4.411964	-1.902681
14	0.203175	-1.078137	-3.852083
1	-0.036907	-5.156875	-3.169229
1	-0.039262	-1.840519	-5.108240
1	0.036907	5.156875	3.169229
1	0.039262	1.840519	5.108240
1	-0.039262	-1.840519	5.108240
1	-0.036907	-5.156875	3.169229
1	0.068958	-6.981071	0.000000
1	0.039262	1.840519	-5.108240
1	0.036907	5.156875	-3.169229
1	-0.068958	6.981071	0.000000

M05-2X/TZVP = -4637.769935 Hartree

Low frequencies (cm^{-1}): 29.3194 46.5376 51.0379 69.3818 71.8898 79.3672
96.8439 98.3103 102.7157 104.3471

$Si_{22}H_{12}$:

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-4.111327	3.715454	0.213552

14	-0.375717	2.927888	0.257785
14	3.373929	2.138300	0.269191
14	-2.070409	4.400735	-0.182455
14	-4.586661	1.529408	-0.257692
14	1.699278	3.596711	-0.170014
14	-0.819600	0.742458	-0.239891
14	2.932069	-0.039380	-0.196267
14	-6.654888	0.811671	0.164000
14	-2.932069	0.039380	0.196267
14	0.819600	-0.742458	0.239891
14	-7.108515	-1.347523	-0.207698
14	-3.373929	-2.138300	-0.269191
14	0.375717	-2.927888	-0.257785
14	-5.482478	-2.807932	0.158843
14	-1.699278	-3.596711	0.170014
1	-5.786827	-4.246237	-0.074311
1	-2.014450	-5.028827	-0.096417
1	2.014450	5.028827	0.096417
1	-1.738797	5.831066	0.064589
14	2.070409	-4.400735	0.182455
1	1.738797	-5.831066	-0.064589
14	4.111327	-3.715454	-0.213552
1	5.236461	-4.666361	0.004958
14	5.482478	2.807932	-0.158843
1	5.786827	4.246237	0.074311
14	7.108515	1.347523	0.207698
1	8.511241	1.794719	-0.007214
14	6.654888	-0.811671	-0.164000
14	4.586661	-1.529408	0.257692
1	7.767856	-1.775967	0.054521
1	-5.236461	4.666361	-0.004958
1	-7.767856	1.775967	-0.054521
1	-8.511241	-1.794719	0.007214

M05-2X/TZVP = -6375.9245312 Hartree

Low frequencies (cm^{-1}): 13.6254 31.0127 40.2797 51.8485 55.9957 62.4569
73.3796 74.5823 79.2108 81.8822

$Si_{28}H_{14}$:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
14	-5.975407	4.116295	0.361829
14	-2.240676	3.323331	0.332292
14	1.510510	2.533197	0.287711
14	-3.940839	4.809015	-0.046654
14	-6.461388	1.939751	-0.150163
14	-0.178123	4.002438	-0.108124
14	-2.700238	1.143717	-0.205869
14	1.055360	0.353206	-0.222315
14	-8.518650	1.220771	0.298471
14	-4.799478	0.440082	0.257675
14	-1.055360	-0.353206	0.222315
14	-8.990900	-0.936895	-0.099264
14	-5.258232	-1.734404	-0.22618
14	-1.510510	-2.533197	-0.287711
14	-7.369632	-2.404906	0.224605

14	-3.594741	-3.201373	0.167834
1	-7.676115	-3.839798	-0.025531
1	-3.912458	-4.627791	-0.124629
1	0.141385	5.425525	0.197663
1	-3.601752	6.230926	0.234715
14	0.178123	-4.002438	0.108124
1	-0.141385	-5.425525	-0.197663
14	2.240676	-3.323331	-0.332292
14	3.594741	3.201373	-0.167834
1	3.912458	4.627791	0.124629
14	5.258232	1.734404	0.226183
14	4.799478	-0.440082	-0.257675
14	2.700238	-1.143717	0.205869
1	-7.105178	5.070398	0.185871
1	-9.635639	2.187943	0.115754
1	-10.393712	-1.376335	0.129726
14	3.940839	-4.809015	0.046654
1	3.601752	-6.230926	-0.234715
14	5.975407	-4.116295	-0.361829
1	7.105178	-5.070398	-0.185871
14	6.461388	-1.939751	0.150163
14	8.518650	-1.220771	-0.298471
14	7.369632	2.404906	-0.224605
14	8.990900	0.936895	0.099264
1	7.676115	3.839798	0.025531
1	10.393712	1.376335	-0.129726
1	9.635639	-2.187943	-0.115754

M05-2X/TZVP = -8114.0770256 Hartree

Low frequencies (cm^{-1}): 10.8584 23.9840 29.3546 44.2029 44.2662 47.5657
53.4402 57.3382 64.3312 68.8955

$Si_{24}H_{12}$:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
1	-0.739014	7.218280	-0.044875
1	-4.173846	5.933605	0.042744
1	5.880945	4.250001	0.050054
1	3.051413	6.581974	-0.046517
1	-7.226330	-0.646734	-0.049769
1	-6.619547	2.969427	0.042541
1	7.226445	0.646801	0.047213
1	6.619519	-2.969585	-0.044384
1	4.173991	-5.933134	-0.044525
1	0.739041	-7.218064	0.042320
1	-5.880831	-4.249652	-0.052325
1	-3.051356	-6.581793	0.043723
14	-5.855604	-0.118080	0.195049
14	-2.086014	-0.779170	0.238914
14	-4.154576	-1.551758	-0.235018
14	-5.495700	2.021856	-0.195723
14	-1.717443	1.416351	-0.235229
14	-3.420950	2.822092	0.236635
14	0.368546	2.195377	0.237809
14	4.154860	1.551748	0.235163
14	4.500064	3.748917	-0.194417

14	2.824803	5.129307	0.192013
14	0.732514	4.373487	-0.234475
14	-0.997403	5.771398	0.196350
14	-3.029683	5.010794	-0.197168
14	1.717307	-1.416261	0.236477
14	2.086019	0.779265	-0.237379
14	-0.368679	-2.195505	-0.236446
14	-4.500055	-3.749101	0.194022
14	-2.824615	-5.128999	-0.194233
14	-0.732621	-4.373775	0.235735
14	0.997311	-5.770994	-0.198178
14	3.029621	-5.011020	0.197178
14	3.420792	-2.821984	-0.235383
14	5.495989	-2.021979	0.195142
14	5.855485	0.117954	-0.195853

M05-2X/TZVP = -6954.9397408 Hartree

Low frequencies (cm^{-1}): 21.5640 25.0996 28.3627 49.6839 55.6295 72.9210
73.4379 74.3821 78.7502 89.4998

$Si_{30}H_{14}$:

Atomic Number		Coordinates (Angstroms)		
		X	Y	Z
1	14	0	-0.176723	4.395497	3.844711
2	14	0	-0.229270	1.103724	1.925756
3	14	0	-0.264759	-2.207615	0.000000
4	14	0	0.255581	2.223248	3.864797
5	14	0	0.258794	5.537385	1.928552
6	14	0	0.229270	-1.103724	1.925756
7	14	0	0.264759	2.207615	0.000000
8	14	0	0.229270	-1.103724	-1.925756
9	14	0	-0.184184	7.736055	1.903499
10	14	0	-0.203013	4.429775	0.000000
11	14	0	-0.229270	1.103724	-1.925756
12	14	0	0.174054	8.832457	0.000000
13	14	0	0.258794	5.537385	-1.928552
14	14	0	0.255581	2.223248	-3.864797
15	14	0	-0.184184	7.736055	-1.903499
16	14	0	-0.176723	4.395497	-3.844711
17	1	0	0.054403	8.482914	-3.168965
18	1	0	0.085891	5.147615	-5.104428
19	14	0	-0.195288	1.076048	-5.796175
20	1	0	0.039158	1.841305	-7.051883
21	14	0	0.195288	-1.076048	-5.796175
22	1	0	-0.039158	-1.841305	-7.051883
23	14	0	0.203013	-4.429775	0.000000
24	14	0	-0.258794	-5.537385	-1.928552
25	14	0	0.176723	-4.395497	-3.844711
26	14	0	-0.255581	-2.223248	-3.864797
27	1	0	-0.085891	-5.147615	-5.104428
28	1	0	0.085891	5.147615	5.104428
29	1	0	0.054403	8.482914	3.168965
30	1	0	-0.047234	10.304032	0.000000
31	14	0	-0.195288	1.076048	5.796175
32	14	0	0.184184	-7.736055	-1.903499
33	1	0	-0.054403	-8.482914	-3.168965
34	14	0	-0.174054	-8.832457	0.000000

35	14	0	0.184184	-7.736055	1.903499
36	14	0	-0.258794	-5.537385	1.928552
37	14	0	0.176723	-4.395497	3.844711
38	14	0	-0.255581	-2.223248	3.864797
39	14	0	0.195288	-1.076048	5.796175
40	1	0	0.047234	-10.304032	0.000000
41	1	0	-0.054403	-8.482914	3.168965
42	1	0	-0.085891	-5.147615	5.104428
43	1	0	-0.039158	-1.841305	7.051883
44	1	0	0.039158	1.841305	7.051883

M05-2X/TZVP = -8693.083514 Hartree

Low frequencies (cm^{-1}): 14.8551 25.9361 26.3614 32.3294 40.1312 58.3722
61.7233 64.6167 67.3160 68.0219

$Si_{34}H_{16}$:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
14	-7.857162	4.504252	0.372302
14	-4.123086	3.712799	0.351218
14	-0.368893	2.929226	0.332408
14	-5.821356	5.204789	-0.013906
14	-8.338853	2.333115	-0.169172
14	-2.059555	4.403278	-0.053645
14	-4.578646	1.538808	-0.223355
14	-0.820095	0.751048	-0.213286
14	-10.393313	1.607919	0.269884
14	-6.674351	0.831423	0.230285
14	-2.931136	0.040940	0.206058
14	-10.869468	-0.549731	-0.143625
14	-7.135382	-1.342180	-0.267875
14	-3.383004	-2.138110	-0.314454
14	-9.251105	-2.018250	0.172922
14	-5.479186	-2.809543	0.118870
1	-9.552356	-3.452454	-0.086417
1	-5.788856	-4.234031	-0.19058
1	-1.746946	5.817887	0.294894
1	-5.485557	6.620386	0.300223
14	-1.711066	-3.610629	0.083786
1	-2.021356	-5.028979	-0.252010
14	0.368893	-2.929226	-0.332408
14	1.711066	3.610629	-0.083786
1	2.021356	5.028979	0.252010
14	3.383004	2.138110	0.314454
14	2.931136	-0.040940	-0.206058
14	0.820095	-0.751048	0.213286
1	-8.988384	5.458557	0.208070
1	-11.512134	2.574975	0.098456
1	-12.273558	-0.986508	0.081991
14	2.059555	-4.403278	0.053645
1	1.746946	-5.817887	-0.294894
14	4.123086	-3.712799	-0.351218
14	4.578646	-1.538808	0.223355
14	6.674351	-0.831423	-0.230285
14	5.479186	2.809543	-0.118870
14	7.135382	1.342180	0.267875

1	5.788856	4.234031	0.190583
14	5.821356	-5.204789	0.013906
14	7.857162	-4.504252	-0.372302
14	8.338853	-2.333115	0.169172
14	9.251105	2.018250	-0.172922
1	9.552356	3.452454	0.086417
14	10.869468	0.549731	0.143625

M05-2X/TZVP = -9852.2284112 Hartree

Low frequencies (cm^{-1}): 5.5334 18.4470 20.2671 33.0483 36.3724 38.0824
42.0703 48.9417 51.9087 58.2302

$Si_{38}H_{16}$:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
14	-4.203177	5.971668	0.184738
14	-0.549554	4.839366	0.260330
14	3.126173	3.709145	0.283914
14	-2.104923	6.463355	-0.177644
14	-4.878244	3.829519	-0.271266
14	1.570117	5.317391	-0.147856
14	-1.199505	2.695389	-0.239130
14	2.480027	1.566758	-0.195125
14	-6.987199	3.315081	0.157820
14	-3.344731	2.194155	0.210373
14	0.316840	1.065478	0.250854
14	-7.669316	1.186524	-0.273833
14	-3.986150	0.062418	-0.288814
14	-0.316840	-1.065478	-0.250854
14	-6.148575	-0.441089	0.179861
14	-2.480027	-1.566758	0.195125
1	2.016927	6.714864	0.112902
1	-1.645112	7.859730	0.056544
14	1.199505	-2.695389	0.239130
14	3.344731	-2.194155	-0.210373
14	5.258926	4.180279	-0.156814
1	5.705642	5.578518	0.100805
14	6.796600	2.574308	0.264480
14	6.148575	0.441089	-0.179861
14	3.986150	-0.062418	0.288814
1	-5.234618	7.020156	-0.041717
1	-8.010481	4.370221	-0.084966
14	4.878244	-3.829519	0.271266
14	6.987199	-3.315081	-0.157820
1	8.010481	-4.370221	0.084966
14	7.669316	-1.186524	0.273833
14	9.800145	-0.668081	-0.17820
14	8.952746	3.043483	-0.186651
14	10.447198	1.438941	0.165838
1	9.393079	4.447138	0.039725
1	11.881485	1.765392	-0.056030
1	10.816747	-1.731459	0.044358
14	4.203177	-5.971668	-0.184738
14	2.104923	-6.463355	0.177644
14	0.549554	-4.839366	-0.260330

14	-1.570117	-5.317391	0.147856
14	-3.126173	-3.709145	-0.283914
14	-5.258926	-4.180279	0.156814
14	-6.796600	-2.574308	-0.264480
14	-10.447198	-1.438941	-0.165838
14	-9.800145	0.668081	0.178201
14	-8.952746	-3.043483	0.186651
1	5.234618	-7.020156	0.041717
1	1.645112	-7.859730	-0.056544
1	-2.016927	-6.714864	-0.112902
1	-5.705642	-5.578518	-0.100805
1	-9.393079	-4.447138	-0.039725
1	-11.881485	-1.765392	0.056030
1	-10.816747	1.731459	-0.044358

M05-2X/TZVP = -11010.2401471 Hartree

Low frequencies (cm^{-1}): 13.5474 21.0937 26.5892 30.6355 34.3365 45.2027
48.6786 51.4115 53.1512
66.1835

$Si_{46}H_{18}$:

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-6.729007	-5.803244	-0.217296
14	-2.974044	-5.093611	-0.245602
14	0.803236	-4.399248	-0.271637
14	-4.707565	-6.530199	0.184077
14	-7.163608	-3.606630	0.267671
14	-0.929228	-5.813454	0.179238
14	-3.383686	-2.894013	0.266355
14	0.399385	-2.195556	0.210460
14	-9.191074	-2.849698	-0.184924
14	-5.450584	-2.149780	-0.187044
14	-1.687550	-1.448002	-0.218837
14	-9.638670	-0.666353	0.282173
14	-5.856331	0.040054	0.317650
14	-2.080361	0.744431	0.272415
14	-7.943684	0.786224	-0.152457
14	-4.176815	1.490926	-0.157585
1	-0.649304	-7.253125	-0.086401
1	-4.403565	-7.968566	-0.051428
14	-0.399385	2.195556	-0.210460
14	1.687550	1.448002	0.218837
14	2.861744	-5.109429	0.168545
1	3.142586	-6.550027	-0.092094
14	4.576867	-3.695293	-0.298020
14	4.176815	-1.490926	0.157585
14	2.080361	-0.744431	-0.272415
1	-7.875930	-6.730541	-0.010530
1	-10.331426	-3.786498	0.025623
14	3.383686	2.894013	-0.266355
14	5.450584	2.149780	0.187044
14	5.856331	-0.040054	-0.317650
14	7.943684	-0.786224	0.152457

14	6.650690	-4.395472	0.153994
14	8.349529	-2.978768	-0.289088
1	6.934260	-5.838220	-0.090748
14	2.974044	5.093611	0.245602
14	0.929228	5.813454	-0.179238
14	-0.803236	4.399248	0.271637
14	-2.861744	5.109429	-0.168545
14	-4.576867	3.695293	0.298020
14	-6.650690	4.395472	-0.153994
14	-8.349529	2.978768	0.289088
14	-12.105709	2.261936	0.171134
14	-11.686926	0.094887	-0.186838
14	-10.442633	3.686119	-0.168376
1	0.649304	7.253125	0.086401
1	-3.142586	6.550027	0.092094
1	-6.934260	5.838220	0.090748
1	-10.720044	5.132411	0.047414
1	-13.494420	2.738158	-0.068589
1	-12.821822	-0.848795	0.007659
14	4.707565	6.530199	-0.184077
1	4.403565	7.968566	0.051428
14	6.729007	5.803244	0.217296
14	7.163608	3.606630	-0.267671
14	9.191074	2.849698	0.184924
1	10.331426	3.786498	-0.025623
14	9.638670	0.666353	-0.282173
14	10.442633	-3.686119	0.168376
1	10.720044	-5.132411	-0.047414
14	11.686926	-0.094887	0.186838
1	12.821822	0.848795	-0.007659
14	12.105709	-2.261936	-0.171134
1	13.494420	-2.738158	0.068589
1	7.875930	6.730541	0.010530

M05-2X/TZVP = -13327.3952803 Hartree

Low frequencies (cm^{-1}): 3.9000 15.1412 16.9984 27.0877 28.8444 31.2838
36.4608 41.3246 43.2622 49.8481

$Si_{48}H_{18}$:

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.173322	4.391100	5.784552
14	-0.233605	1.095758	3.860974
14	-0.260676	-2.215855	1.932112
14	0.251705	2.223170	5.801388
14	0.269248	5.546137	3.867792
14	0.233605	-1.095758	3.860974
14	0.260676	2.215855	1.932112
14	0.225210	-1.110702	0.000000
14	-0.179248	7.724049	3.843104
14	-0.205578	4.425148	1.928365
14	-0.225210	1.110702	0.000000
14	0.254874	8.860596	1.929888
14	0.280304	5.530347	0.000000
14	0.260676	2.215855	-1.932112
14	-0.199136	7.747794	0.000000
14	-0.205578	4.425148	-1.928365
14	-0.233605	1.095758	-3.860974

14	0.233605	-1.095758	-3.860974
14	0.205578	-4.425148	1.928365
14	-0.280304	-5.530347	0.000000
14	0.205578	-4.425148	-1.928365
14	-0.260676	-2.215855	-1.932112
1	0.083251	5.142876	7.045636
1	0.079106	8.476838	5.103318
14	-0.251705	-2.223170	-5.801388
14	0.173322	-4.391100	-5.784552
1	-0.083251	-5.142876	-7.045636
14	-0.269248	-5.546137	-3.867792
14	0.179248	-7.724049	-3.84310
14	0.199136	-7.747794	0.000000
14	-0.254874	-8.860596	-1.929888
1	-0.079106	-8.476838	-5.103318
14	0.193429	-1.075784	-7.734899
14	-0.193429	1.075784	-7.734899
14	0.251705	2.223170	-5.801388
14	-0.173322	4.391100	-5.784552
14	0.269248	5.546137	-3.867792
14	-0.179248	7.724049	-3.843104
14	0.254874	8.860596	-1.929888
14	0.150016	12.159344	0.000000
14	-0.201481	11.059546	1.902415
1	-0.201481	11.059546	-1.902415
1	-0.037324	-1.843382	-8.989704
1	0.037324	1.843382	-8.989704
1	0.083251	5.142876	-7.045636
1	0.079106	8.476838	-5.103318
1	0.028548	11.806860	-3.169161
1	-0.080702	13.629376	0.000000
1	0.028548	11.806860	3.169161
14	-0.193429	1.075784	7.734899
14	-0.251705	-2.223170	5.801388
14	-0.269248	-5.546137	3.867792
14	-0.254874	-8.860596	1.929888
14	0.201481	-11.059546	-1.902415
14	-0.150016	-12.159344	0.000000
14	0.193429	-1.075784	7.734899
14	0.173322	-4.391100	5.784552
14	0.179248	-7.724049	3.843104
14	0.201481	-11.059546	1.902415
1	0.037324	1.843382	8.989704
1	-0.037324	-1.843382	8.989704
1	-0.083251	-5.142876	7.045636
1	-0.079106	-8.476838	5.103318
1	-0.028548	-11.806860	3.169161
1	0.080702	-13.629376	0.000000
1	-0.028548	-11.806860	-3.169161

M05-2X/TZVP = -13906.4007131 Hartree

Low frequencies (cm^{-1}): 10.7755 16.0019 17.7092 20.0068 26.6434 34.6886
40.6651 43.4322 44.7646 50.1937

$Si_{58}H_{20}$:

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
14	-0.278896	2.728535	6.753585
14	-0.324457	-0.566148	4.823633
14	0.150304	0.561856	6.766923
14	0.164071	3.889427	4.839776
14	0.189824	0.561223	2.903202
14	-0.288441	6.063391	4.817963
14	-0.289420	2.762619	2.894128
14	0.183936	7.210126	2.912921
14	0.230211	3.875543	0.975649
14	-0.280151	9.393543	2.873409
14	-0.242280	6.088289	0.963294
14	-0.209435	2.767896	-0.96893
14	0.258245	0.552393	-0.960719
14	0.152917	-2.754299	4.825730
14	-0.310807	-3.879496	2.889286
14	0.209435	-2.767896	0.968937
14	-0.258245	-0.552393	0.960719
14	-0.189824	-0.561223	-2.903202
14	0.289420	-2.762619	-2.894128
14	-0.230211	-3.875543	-0.975649
14	0.242280	-6.088289	-0.963294
14	0.173465	-6.082154	2.892154
14	-0.275223	-7.193953	0.954686
14	0.324457	0.566148	-4.823633
14	-0.152917	2.754299	-4.825730
14	0.310807	3.879496	-2.889286
14	-0.173465	6.082154	-2.892154
14	0.275223	7.193953	-0.954686
14	-0.219422	9.407059	-0.965847
14	0.192701	10.522957	0.972943
14	-0.272636	12.725313	0.930058
14	-0.150304	-0.561856	-6.766923
14	0.278896	-2.728535	-6.753585
14	-0.164071	-3.889427	-4.839776
14	0.288441	-6.063391	-4.817963
1	0.031054	-6.811279	-6.081534
14	-0.183936	-7.210126	-2.912921
14	0.219422	-9.407059	0.965847
14	0.280151	-9.393543	-2.873409
1	0.038594	-10.145457	-4.137814
14	-0.192701	-10.522957	-0.972943
1	0.022621	-3.477320	-8.016504
14	-0.289134	-0.587040	8.700740
14	-0.334668	-3.883338	6.764558
14	-0.324742	-7.204945	4.824384
14	-0.267762	-10.522725	2.886349
14	0.272636	-12.725313	-0.930058
1	0.071787	-13.474547	-2.200739
14	0.109571	13.823582	-0.963333
14	0.267762	10.522725	-2.886349
14	0.324742	7.204945	-4.824384
14	0.334668	3.883338	-6.764558
14	0.289134	0.587040	-8.700740
1	0.061171	-0.181096	-9.955686
14	-0.109571	-13.823582	0.963333
1	0.129342	-15.292231	0.972758
14	0.103287	-2.737449	8.700432
14	0.127527	-9.381020	4.806409

14	0.201854	-12.716729	2.872488
14	-0.201854	12.716729	-2.872488
14	-0.127527	9.381020	-4.806409
14	-0.094487	6.050137	-6.746466
14	-0.103287	2.737449	-8.700432
14	0.094487	-6.050137	6.746466
1	0.043572	13.463662	-4.136457
1	0.133074	10.135521	-6.064932
1	0.157545	6.806371	-8.005661
1	0.124754	3.508248	-9.953707
1	-0.124754	-3.508248	9.953707
1	-0.157545	-6.806371	8.005661
1	-0.133074	-10.135521	6.064932
1	-0.043572	-13.463662	4.136457
1	-0.061171	0.181096	9.955686
1	-0.022621	3.477320	8.016504
1	-0.031054	6.811279	6.081534
1	-0.038594	10.145457	4.137814
1	-0.071787	13.474547	2.200739
1	-0.129342	15.292231	-0.972758

M05-2X/TZVP = -16802.5602758 Hartree

Low frequencies (cm^{-1}):

$Si_{70}H_{22}$:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
14	-0.172292	4.389529	7.718518
14	-0.234459	1.094447	5.792029
14	-0.256273	-2.222484	3.863912
14	0.248438	2.221483	7.733694
14	0.259530	5.547375	5.800385
14	0.234459	-1.094447	5.792029
14	0.256273	2.222484	3.863912
14	0.232614	-1.106221	1.933107
14	-0.179132	7.723401	5.781457
14	-0.219508	4.422776	3.860707
14	-0.232614	1.106221	1.933107
14	0.262705	8.869837	3.868362
14	0.270312	5.538657	1.933473
14	0.250480	2.212783	0.000000
14	-0.202774	7.748525	1.928225
14	-0.209731	4.429339	0.000000
14	-0.232614	1.106221	-1.933107
14	0.232614	-1.106221	-1.933107
14	0.219508	-4.422776	3.860707
14	-0.270312	-5.538657	1.933473
14	0.209731	-4.429339	0.000000
14	-0.250480	-2.212783	0.000000
1	0.083222	5.140733	8.979995
1	0.082381	8.472598	7.043107
14	-0.256273	-2.222484	-3.863912
14	0.219508	-4.422776	-3.860707
14	-0.270312	-5.538657	-1.933473
14	0.202774	-7.748525	-1.928225
14	0.202774	-7.748525	1.928225
14	-0.282714	-8.856318	0.000000

14	0.234459	-1.094447	-5.792029
14	-0.234459	1.094447	-5.792029
14	0.256273	2.222484	-3.863912
14	-0.219508	4.422776	-3.860707
14	0.270312	5.538657	-1.933473
14	-0.202774	7.748525	-1.928225
14	0.282714	8.856318	0.000000
14	0.246931	12.186085	1.930843
14	-0.190524	11.054138	3.840303
14	-0.204684	11.070611	0.000000
1	0.068813	11.803807	5.102209
14	-0.248438	-2.221483	-7.733694
14	0.172292	-4.389529	-7.718518
14	-0.259530	-5.547375	-5.800385
14	0.179132	-7.723401	-5.781457
1	-0.082381	-8.472598	-7.043107
14	-0.262705	-8.869837	-3.868362
14	0.204684	-11.070611	0.000000
14	0.190524	-11.054138	-3.840303
1	-0.068813	-11.803807	-5.102209
14	-0.246931	-12.186085	-1.930843
1	-0.083222	-5.140733	-8.979995
14	-0.193249	1.075699	9.668804
1	0.036757	1.844696	10.922784
14	-0.248438	-2.221483	7.733694
14	-0.259530	-5.547375	5.800385
14	-0.262705	-8.869837	3.868362
14	-0.246931	-12.186085	1.930843
14	0.211371	-14.387562	-1.901854
1	-0.019551	-15.133449	-3.169238
14	0.246931	12.186085	-1.930843
14	0.262705	8.869837	-3.868362
14	0.259530	5.547375	-5.800385
14	0.248438	2.221483	-7.733694
14	0.193249	-1.075699	-9.668804
1	-0.036757	-1.844696	-10.922784
14	-0.211371	14.387562	1.901854
1	0.019551	15.133449	3.169238
14	0.143291	15.487147	0.000000
1	-0.086429	16.957278	0.000000
14	-0.143291	-15.487147	0.000000
1	0.086429	-16.957278	0.000000
14	0.193249	-1.075699	9.668804
14	0.172292	-4.389529	7.718518
14	0.190524	-11.054138	3.840303
14	0.211371	-14.387562	1.901854
14	-0.211371	14.387562	-1.901854
14	-0.190524	11.054138	-3.840303
14	-0.179132	7.723401	-5.781457
14	-0.172292	4.389529	-7.718518
14	-0.193249	1.075699	-9.668804
14	0.179132	-7.723401	5.781457
1	0.019551	15.133449	-3.169238
1	0.068813	11.803807	-5.102209
1	0.082381	8.472598	-7.043107
1	0.083222	5.140733	-8.979995
1	0.036757	1.844696	-10.922784
1	-0.036757	-1.844696	10.922784
1	-0.083222	-5.140733	8.979995

1	-0.082381	-8.472598	7.043107
1	-0.068813	-11.803807	5.102209
1	-0.019551	-15.133449	3.169238

M05-2X/TZVP = -20277.7242274 Hartree

Low frequencies (cm^{-1}): 7.9186 10.8206 12.4838 13.9767 17.1679 22.5292
27.6012 29.8534 31.6339 35.5556

PBE1PBE/6-311+G(d,p)

Si_6H_6:

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.000000	3.669212	0.042970
1	3.177631	1.834606	-0.042970
1	3.177631	-1.834606	0.042970
1	0.000000	-3.669212	-0.042970
1	-3.177631	-1.834606	0.042970
1	-3.177631	1.834606	-0.042970
14	-1.902083	-1.098168	-0.177914
14	0.000000	-2.196336	0.177914
14	1.902083	-1.098168	-0.177914
14	1.902083	1.098168	0.177914
14	0.000000	2.196336	-0.177914
14	-1.902083	1.098168	0.177914

PBE1PBE/6-311+G(d,p) = -1739.7900893 Hartree

Low frequencies (cm^{-1}): 100.9010 100.9011 124.0246 146.1210 146.1222 209.9951
368.1760 387.3672 387.3726 387.7599.

$Si_{10}H_{14}$ (A):

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.251142	2.205317	3.864151
14	0.215942	2.200431	0.000000
14	0.251142	2.205317	-3.864151
14	0.398068	1.052031	5.736021
14	0.398068	1.064316	1.919357
14	0.398068	1.064316	-1.919357
14	-0.398068	-1.052031	5.736021
14	-0.398068	-1.064316	1.919357
14	-0.398068	-1.064316	-1.919357
14	-0.251142	-2.205317	3.864151
14	-0.215942	-2.200431	0.000000
1	-0.793078	-3.593055	3.857294
1	-0.777192	-3.582145	0.000000
14	-0.251142	-2.205317	-3.864151
1	-0.793078	-3.593055	-3.857294
14	-0.398068	-1.052031	-5.736021
1	-0.356450	-1.788296	-7.030095
14	0.398068	1.052031	-5.736021
1	0.356450	1.788296	7.030095
1	-0.356450	-1.788296	7.030095
1	0.356450	1.788296	-7.030095
1	0.793078	3.593055	3.857294
1	0.777192	3.582145	0.000000

1	0.793078	3.593055	-3.857294

PBE1PBE/6-311+G(d,p) = -4057.1951243 Hartree

Low frequencies (cm^{-1}): 20.9883 35.1994 53.5056 59.7313 73.5560 77.7626 90.8391 99.8520 106.6263 107.2382.

$Si_{18}H_{12}$ (A):

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	3.690464	0.672552	0.000096
6	2.497484	1.361453	0.000093
6	1.256151	0.698041	0.000004
6	1.246272	-0.715003	-0.000042
6	2.478069	-1.395587	-0.000041
6	3.680600	-0.723411	0.000018
6	-0.003695	1.436792	-0.000020
6	-0.023479	-1.436526	-0.000048
6	-1.242277	-0.721626	0.000042
6	-1.232334	0.738657	0.000038
6	-2.447738	-1.447966	0.000108
6	-2.466879	-2.825469	0.000061
6	-1.262768	-3.531776	-0.000063
6	-0.069514	-2.843109	-0.000112
1	4.629820	1.215430	0.000171
1	4.612294	-1.279345	0.000018
1	-3.414109	-3.354481	0.000114
1	-1.262163	-4.616743	-0.000116
6	-0.030532	2.843882	-0.000105
6	-1.214127	3.548823	-0.000095
6	-2.427869	2.859020	0.000001
6	-2.427701	1.481394	0.000058
1	-1.198964	4.633681	-0.000168
1	-3.367843	3.400860	0.000016
1	-3.381607	0.969864	0.000109
1	-3.394652	-0.923541	0.000198
1	0.850144	-3.414086	-0.000203
1	2.497534	-2.477867	-0.000075
1	2.531936	2.443362	0.000182
1	0.896866	3.402018	-0.000201

PBE1PBE/6-311+G(d,p) = -692.5131535 Hartree
Low frequencies (cm^{-1}): 52.7854 52.9619 105.2069 120.6883 261.0411 261.2936 272.1419 272.1950 410.6721 410.7266.

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Table 1. *The buckling frequency, scattering activity, enhancement in scattering activity and binding energy for silicene fragments in the presence of metal clusters at PBE1PBE/6-311+G(d,p) level of theory.*

Species	Buckling Frequency (cm^{-1})	Scattering Acitvity (S. A) (A^4/AMU)	Enhancement in S.A	Binding Energy (kcal/mol)	Induced Polarizability (a.u)	HOMO-LUMO gap (eV)
Si_6H_6	124	4.01				3.52
$Si_6H_6...Au_2$	83	23.22	5.79	-23.77	13.73	3.23
$Si_6H_6...Au_4$	72	49.66	12.38	-20.12	47.41	1.98
$Si_6H_6...Au_{20}$	83	118.21	29.48	-23.82	87.03	2.66
$Si_6H_6...Ag_2$	91	65.56	16.35	-13.98	16.18	1.82
$Si_6H_6...Ag_4$	68	160.1	39.93	-10.71	46.92	1.28
$Si_6H_6...Ag_{20}$	94	167.93	41.88	-14.40	80.59	1.76
$Si_{14}H_{10}$	145	46.67				1.87
$Si_{14}H_{10}...Au_2$	130	82.07	1.76	-22.49	14.51	1.76
$Si_{14}H_{10}...Ag_2$	134	96.28	2.06	-14.86	28.1	1.41
$Si_{18}H_{12}$	145	27.56				2.53
$Si_{18}H_{12}...Au_2$	132	62.59	2.27	-20.55	24.05	2.31
$Si_{18}H_{12}..Ag_2$	134	68.58	2.49	-12.2	34.68	1.72

Normal Modes for which Scattering Activity decreased (*PBE1PBE/6-311+G(d,p) level of theory.)*

HSB			HSB…Au_2		HSB...Au_4		HSB...Au_{20}	
Normal Mode	Frequency	S.A	Frequency	S.A	Frequency	S.A	Frequency	S.A
Ring Expansion	368	167.49	375	146.52	372	108.61	375	122.16
Si-H Wagging	547	3.98	554	0.00	557	0.70	559	0.02
Si-H Wagging	712	46.74	710	35.56	709	36.42	711	25.34
Si-H Wagging	712	46.76	710	35.28	710	38.92	712	24.64
Si-H Asymm. stretching	2224	444.99	2224	435.81	2223	433.82	2223	332.14
Si-H Asymm. stretching	2224	444.66	2224	435.90	2224	426.34	2226	345.41
Si-H symm. stretching	2235	1127.34	2234	1161.1206	2233	1164.05	2233	854.58

Normal Modes for which Scattering Activity increased (*PBE1PBE/6-311+G(d,p) level of theory.)*

HSB			HSB...Au_2		HSB...Au_4		HSB...Au_{20}	
Normal Mode	Frequency	S.A	Frequency	S.A	Frequency	S.A	Frequency	S.A
Si-Si bending (buckling)	101	0	43	9.27	40	3.8183	32	3.36
Si-Si bending	101	0	44	9.47			35	10.98
buckling	124	4.01	83	23.22	72	49.66	83	118.20
Si-H bending	210	0	217	2.44	210	2.73	221	34.09
Si-H bending	387	7.45	376	9.87	376	20.63	388	18.51
Si-H bending	387	7.42	376	8.08	386	10.09	392	16.56
Si-H bending	388	0	399	3.54	393	15.36	406	15.25
Si-H bending	388	0	400	3.37	396	29.06	408	7.78
Si-H bending	396	0	410	3.10	406	2.99	412	5.46
Si-H bending	458	0	458	2.03	457	2.67	459	6.71
Si-H bending	458	0	459	2.00	458	4.44	460	6.85
Si-Si stretching	544	0	550	3.99	548	6.60	550	3.43
Si-H bending	730	0	728	2.56	729	4.77	730	7.75
Si-H bending	730	0	728	2.56	730	3.15	731	7.67
Si-H Asymm. stretching	2221	0	2221	25.67	2220	110.54	2220	171.66
Si-H Asymm. stretching	2230	0	2230	36.92	2229	118.05	2229	230.32
Si-H symm. stretching	2230	0	2230	36.41	2230	116.23	2231	262.73

Normal Modes for which Scattering Activity decreased (*M05-2X/TZVP level of theory.)*

HSB			HSB…Au_2		HSB...Au_4		HSB...Au_{20}	
Normal Mode	Frequency	S.A	Frequency	S.A	Frequency	S.A	Frequency	S.A
Ring Expansion	369	167.65	372	139.61	374	141.68	373	132.20
Si-H Wagging	549	8.92	540	5.21	546	3.12	542	3.37
Si-H Wagging	550	8.92	545	5.40	547	6.19	546	3.65
Si-H Wagging	721	48.65	694	38.28	704	39.65	704	26.83
Si-H Wagging	721	53.14	701	39.44	719	39.25	716	27.48
Si-H Asymm. stretching	2197	519.72	2209	491.94	2199	430.04	2210	328.66
Si-H Asymm. stretching	2197	519.87	2213	616.52	2205	507.32	2220	390.36
Si-H symm. stretching	2207	1393.76	2224	1106.51		1166.86	2227	837.15

Normal Modes for which Scattering Activity increased (*M05-2X/TZVP level of theory.)*

HSB			HSB...Au_2		HSB...Au_4		HSB...Au_{20}	
Normal Mode	Frequency	S.A	Frequency	S.A	Frequency	S.A	Frequency	S.A
Si-Si bending (buckling)	99	0	56	5.97	32	0.68	43	4.59
Si-Si bending	99	0	72	4.06	54	11.28	47	0.62
buckling	125	23.46	104	25.87	96	52.11	100	95.25
Si-H bending	196	0	208	3.46	206	7.26	222	32.52
Si-H bending	395	4.40	378	12.40	388	7.11	402	10.16
Si-H bending	395	4.10	392	2.19	398	13.00	416	9.78
Si-H bending	395	0	396	3.86	401	1.82	420	3.00
Si-H bending	395	0	406	1.80	409	12.27	428	7.49
Si-H bending	401	0	411	0.56	417	3.70	436	6.09
Si-H bending	461	0	454	3.02	457	3.95	462	5.97
Si-H bending	461	0	459	3.18	464	6.98	472	5.81
Si-Si stretching	530	0	534	0.01	542	0.50	538	0.34
Si-H bending	593	0	563	0.00	584	0.19	584	0.03
Si-H bending	623	0.01	600	0.24	617	0.52	619	0.23
Si-H Asymm. stretching	2202	0	2215	41.52	2207	123.75	2221	219.07
Si-H Asymm. stretching	2202	0	2221	124.99	2211	178.49	2225	203.75
Si-H symm. stretching	2207	1393.76	2224	1106.51	2213	1166.86	2227	837.15