Supporting Information on "Open-Shell Singlet Nature and σ-/π-Conjugation Effects on the Third-Order Nonlinear Optical Properties of Si Chains: Polysilane and Poly(disilene-1,2-diyl)"

*Hiroshi Matsui, Kotaro Fukuda, Soichi Ito, Takanori Nagami and Masayoshi Nakano**

Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan

E-mail for M.N.: mnaka@cheng.es.osaka-u.ac.jp

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1. HOMO–LUMO gaps

Table S1. HOMO–LUMO Gaps [a.u.] of $C_\sigma(N)$, $C_\pi(N)$, $Si_\sigma(N)$ and $Si_\pi(N)$ Calculated Using the LC-RBLYP(μ=0.33)/cc-pVDZ Method

N	$C_\sigma(N)$	$C_\pi(N)$	$Si_\sigma(N)$	$Si_\pi(N)$
1	0.573	0.470	0.483	0.283
2	0.546	0.377	0.414	0.229
3	0.536	0.325	0.380	0.199
4	0.527	0.292	0.361	0.181
5	0.521	0.269	0.350	0.169

2. Orbital energy gaps

Table S2. Orbital Energy Gaps [a.u.] between the HOMO and LUMO concerning σ Orbitals of $C_\sigma(N)$, $C_\pi(N)$, $Si_\sigma(N)$ and $Si_\pi(N)$ Calculated Using the LC-RBLYP(μ=0.33)/cc-pVDZ Method

N	$C_\sigma(N)$	$C_\pi(N)$	$Si_\sigma(N)$	$Si_\pi(N)$
1	0.573	0.602	0.483	0.504
2	0.546	0.592	0.414	0.437
3	0.536	0.579	0.380	0.404
4	0.527	0.573	0.361	0.385
5	0.521	0.570	0.350	0.374

3. Excited states

Table S3. Lowest σ-σ* Excited States of $C_\sigma(N)$ and Their Transition, Excitation Energies, and Oscillator Strengths Calculated Using the TD-LC-RBLYP(μ=0.33)/cc-pVDZ Method

N	Major transition	Excitation energy [eV]	Oscillator strength [-]
1	HOMO–1→LUMO+1	11.50	0.193
2	HOMO–3→LUMO	10.15	0.005
3	HOMO→LUMO+1	10.00	0.023
4	HOMO→LUMO+1	9.79	0.014
5	HOMO→LUMO+1	9.66	0.008

Table S4. Lowest σ-σ* Excited States of $C_\pi(N)$ and Their Transition, Excitation Energies, and Oscillator Strengths Calculated Using the TD-LC-RBLYP(μ=0.33)/cc-pVDZ Method

N	Major transition	Excitation energy [eV]	Oscillator strength [-]
1	HOMO–1→LUMO+2	11.82	0.346
2	HOMO–2→LUMO+1	11.21	0.263
3	HOMO–2→LUMO+2	11.12	0.450
4	HOMO–3→LUMO+2	11.11	0.529
5	HOMO–4→LUMO+2	11.09	0.327

Table S5. Lowest σ-σ* Excited States of $Si_\sigma(N)$ and Their Transition, Excitation Energies, and Oscillator Strengths Calculated Using the TD-LC-RBLYP(μ=0.33)/cc-pVDZ Method

N	Major transition	Excitation energy [eV]	Oscillator strength [-]
1	HOMO→LUMO	7.74	0.023
2	HOMO→LUMO	6.75	0.701
3	HOMO→LUMO	6.14	1.652
4	HOMO→LUMO	5.78	2.572

5	HOMO→LUMO	5.57	3.474

Table S6. Lowest σ-σ* Excited States of $Si_\pi(N)$ and Their Transition, Excitation Energies, and Oscillator Strengths Calculated Using the TD-LC-RBLYP(μ=0.33)/cc-pVDZ Method

N	Major transition	Excitation energy [eV]	Oscillator strength [-]
1	HOMO–1→LUMO+1	8.32	0.006
2	HOMO–2→LUMO+2	7.31	0.542
3	HOMO–3→LUMO+3	6.66	0.722
4	HOMO–4→LUMO+3	6.37	2.670
5	HOMO–5→LUMO+4	6.10	2.165

Table S7. Orbital Energy Gaps[a] [a.u.] between the Frontier MOs Concerning the Lowest σ-σ* Excitation[b] of $C_\sigma(N)$, $C_\pi(N)$, $Si_\sigma(N)$ and $Si_\pi(N)$ as a Function of *N*

N	$C_\sigma(N)$	$C_\pi(N)$	$Si_\sigma(N)$	$Si_\pi(N)$
1	0.621	0.627	0.484	0.504
2	0.575	0.591	0.414	0.437
3	0.545	0.579	0.380	0.404
4	0.533	0.573	0.361	0.385
5	0.525	0.570	0.350	0.374

[a] Calculated Using the LC-RBLYP(μ = 0.33)/cc-pVDZ Method.

[b] The MO pair concerning σ-σ* transition is obtained by the TD-LC-RBLYP(μ = 0.33)/cc-pVDZ method.

4. Molecular Orbitals

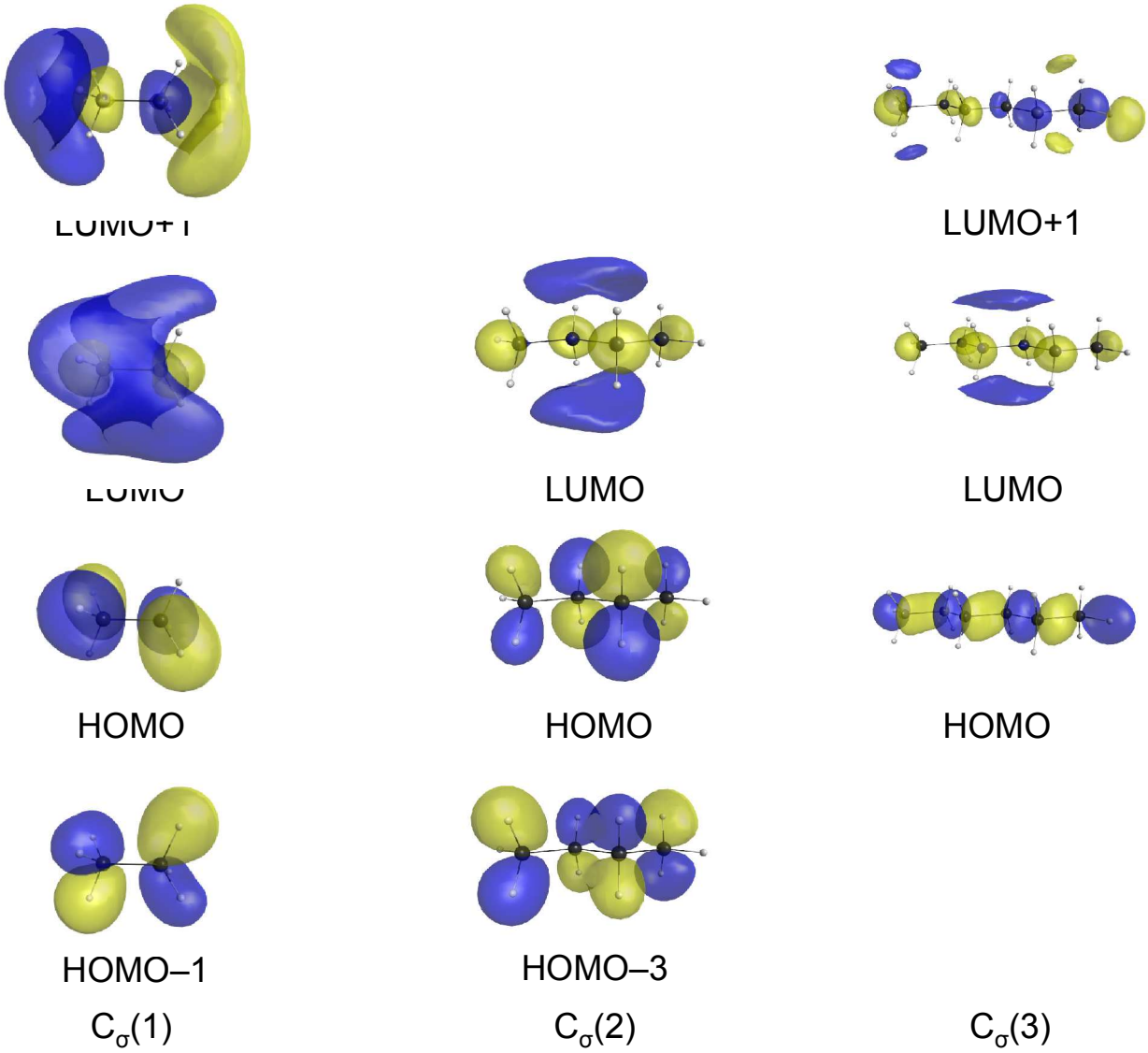

Figure S1. Frontier MOs concerning the lowest σ-σ* excited state of $C_\sigma(N)$ ($1 \leq N \leq 3$) calculated using the LC-RBLYP(μ = 0.33)/cc-pVDZ method. The yellow and blue surfaces indicate the positive and negative isosurfaces with contour value of ±0.04 a.u.

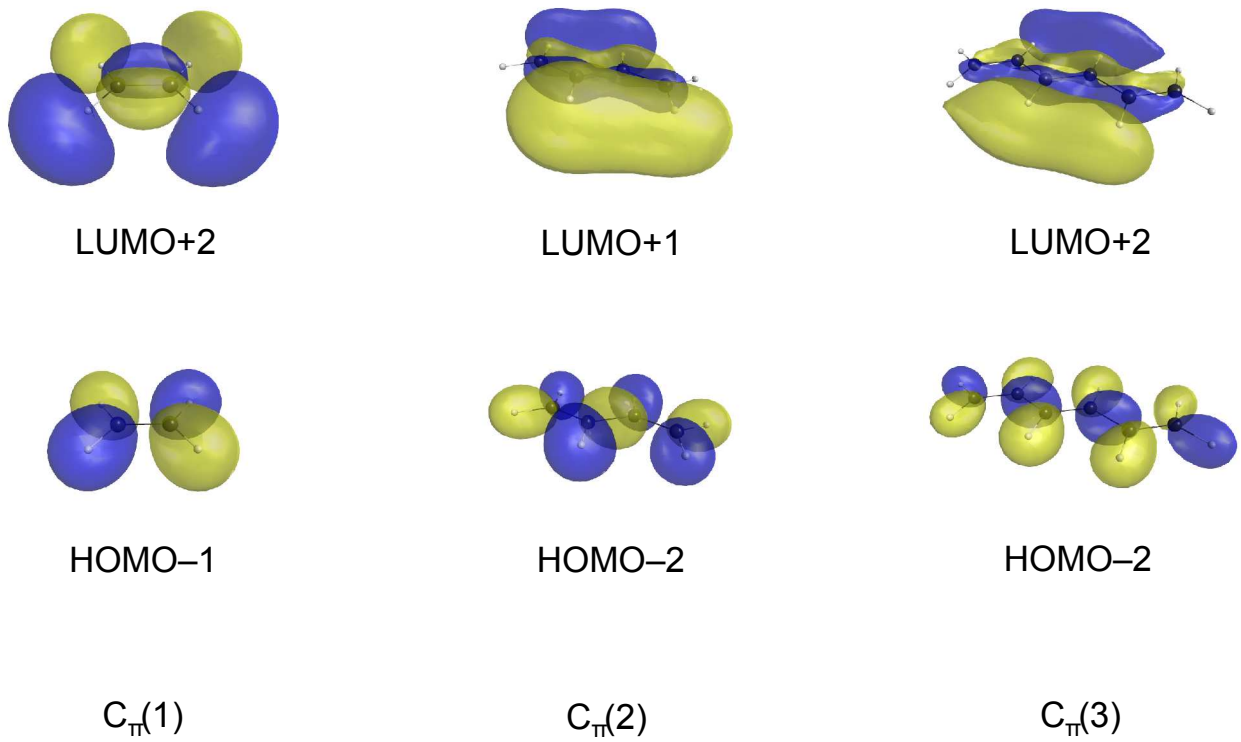

Figure S2. Frontier MOs concerning the lowest σ-σ* excited state of $C_\pi(N)$ ($1 \leq N \leq 3$) calculated using the LC-RBLYP(μ = 0.33)/cc-pVDZ method. The yellow and blue surfaces indicate the positive and negative isosurfaces with contour value of ±0.04 a.u.

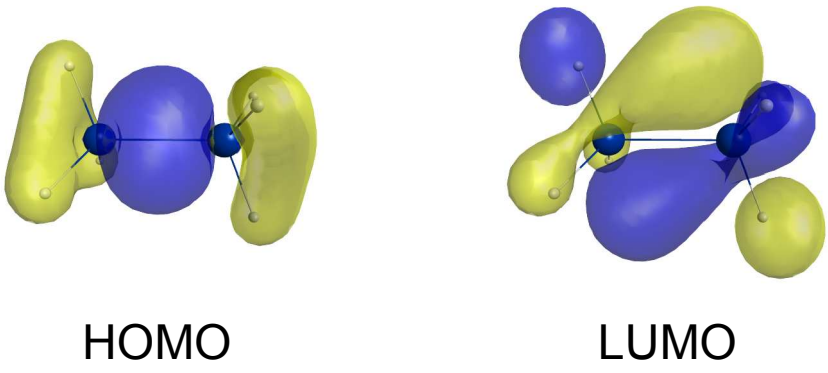

Figure S3. HOMO and LUMO of $Si_\sigma(1)$, which coincide with the frontier MOs concerning the lowest σ-σ* excited state, calculated using the LC-RBLYP(μ = 0.33)/cc-pVDZ method. The yellow and blue surfaces indicate the positive and negative isosurfaces with contour value of ±0.04 a.u.

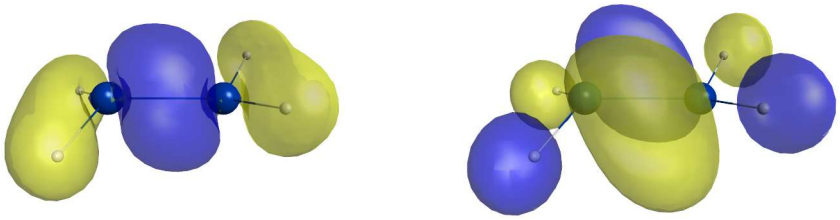

Figure S4. HOMO-1(HOMO(σ)) and LUMO+1(LUMO(σ)) of $Si_\pi(1)$, which are concerned with the lowest σ-σ* excited state, calculated using the LC-RBLYP(μ = 0.33)/cc-pVDZ method. The yellow and blue surfaces indicate the positive and negative isosurfaces with contour value of ±0.04 a.u.

5. Diradical characters of $Si_\pi(N)$

Table S8. Diradical Characters y_i [-] of $Si_\pi(N)$ Calculated Using the PUHF/cc-pVDZ Method

N	y_0	y_1	y_2	y_3	y_4
1	0.077	0.000	0.000	0.000	0.000
2	0.209	0.025	0.000	0.000	0.000
3	0.328	0.053	0.018	0.000	0.000
4	0.422	0.094	0.030	0.016	0.000
5	0.495	0.142	0.048	0.023	0.015

6. γ_{zzzz}/N values

Table S9. γ_{zzzz}/N Values [$\times 10^3$a.u.] of $C_\sigma(N)$, $C_\pi(N)$, $Si_\sigma(N)$ and $Si_\pi(N)$ Calculated Using the LC-UBLYP(μ=0.33)/aug-cc-pVDZ Method

N	$C_\sigma(N)$	$C_\pi(N)$	$Si_\sigma(N)$	$Si_\pi(N)$
1	0.928	0.574	4.50	3.08
2	1.12	2.30	7.65	45.2
3	1.24	7.80	14.5	175
4	1.29	20.6	23.6	470
5	1.34	45.4	33.4	970

7. Optimized structures

Table S10. Optimized Structure of $C_\sigma(1)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	x/Å	y/Å	z/Å
C	0.000000	0.000000	0.764561
C	0.000000	0.000000	-0.764561
H	1.026256	0.000000	1.168468
H	-0.513128	0.888764	1.168468
H	-0.513128	-0.888764	1.168468
H	0.513128	0.888764	-1.168468
H	0.513128	-0.888764	-1.168468
H	-1.026256	0.000000	-1.168468

Table S11. Optimized Structure of $C_\sigma(2)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
C	0.000000	0.000000	1.964846
C	0.547576	0.000000	0.535986
C	-0.547431	-0.000115	-0.535922
C	0.000000	0.000000	-1.964846
H	-0.625960	0.889034	2.153790
H	-0.625887	-0.889087	2.153900
H	0.811641	0.000044	2.710383
H	1.198477	0.882323	0.389492
H	1.198495	-0.882308	0.389600
H	-1.198174	-0.882533	-0.389456
H	-1.198502	0.882071	-0.389363
H	-0.811714	0.000012	-2.710305
H	0.625828	0.889110	-2.153853
H	0.625995	-0.888978	-2.154034

Table S12. Optimized Structure of $C_\sigma(3)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
C	0.000000	0.000000	3.229327
C	0.669647	0.000000	1.853193
C	-0.329387	-0.000301	0.691241
C	0.330260	0.000033	-0.691280
C	-0.669059	-0.000089	-1.852948
C	0.000000	0.000000	-3.229327

H	-0.640431	0.888711	3.362838
H	-0.639702	-0.889221	3.363194
H	0.743913	0.000430	4.042395
H	1.330410	0.882271	1.764220
H	1.330820	-0.881985	1.764452
H	-0.991047	-0.883073	0.780379
H	-0.991751	0.881974	0.780412
H	0.992081	0.882716	-0.780446
H	0.992418	-0.882344	-0.780667
H	-1.329934	-0.882278	-1.763822
H	-1.330041	0.881992	-1.763769
H	-0.744309	-0.000332	-4.042040
H	0.639688	0.889177	-3.363421
H	0.640319	-0.888745	-3.363276

Table S13. Optimized Structure of $C_{\sigma}(4)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
C	0.000000	0.000000	4.504507
C	0.720962	0.000000	3.154488
C	-0.233844	-0.000514	1.955881
C	0.477932	-0.000352	0.599157
C	-0.477135	-0.000693	-0.599074
C	0.234508	-0.000357	-1.955869
C	-0.720545	-0.000498	-3.154282
C	0.000000	0.000000	-4.504507
H	-0.644906	0.888809	4.613686

H	-0.644442	-0.889114	4.613979
H	0.712755	0.000314	5.345042
H	1.384481	0.882313	3.090120
H	1.385018	-0.881933	3.090480
H	-0.898299	-0.883292	2.020032
H	-0.899066	0.881714	2.019871
H	1.142393	0.882243	0.535953
H	1.142964	-0.882519	0.535982
H	-1.141564	-0.883318	-0.535902
H	-1.142195	0.881445	-0.535820
H	0.899073	0.882350	-2.019945
H	0.899602	-0.882655	-2.020127
H	-1.383998	-0.882871	-3.090061
H	-1.384652	0.881365	-3.089765
H	-0.713018	-0.000113	-5.344824
H	0.644315	0.889213	-4.613894
H	0.644969	-0.888701	-4.614206

Table S14. Optimized Structure of $C_\sigma(5)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
C	0.558414	0.000000	1.888715
C	-0.371414	0.000056	0.670738
C	0.369200	0.000068	-0.670733
C	-0.181383	-0.000049	3.230386
C	-0.560345	0.000284	-1.888900
C	0.179963	0.000258	-3.230314

C	0.748531	-0.000267	4.448445
C	0.000000	0.000000	5.783348
C	-0.749308	0.000192	-4.448857
C	0.000000	0.000000	-5.783348
H	1.224340	-0.882355	1.839296
H	1.224315	0.882371	1.839328
H	-1.037321	-0.882276	0.719837
H	-1.037293	0.882417	0.719859
H	1.035216	0.882336	-0.719693
H	1.034992	-0.882355	-0.719811
H	-0.847265	0.882534	3.280761
H	-0.847500	-0.882470	3.280601
H	-1.226385	-0.881993	-1.839776
H	-1.226157	0.882734	-1.839655
H	0.845990	0.882760	-3.280318
H	0.845996	-0.882234	-3.280288
H	1.413233	-0.882578	4.397877
H	1.413761	0.881649	4.397825
H	0.695313	0.000003	6.638366
H	-0.646669	0.889048	5.879271
H	-0.646909	-0.888852	5.879489
H	-1.414368	-0.881867	-4.398559
H	-1.414222	0.882370	-4.398728
H	0.646787	-0.889001	-5.878889
H	-0.694823	-0.000048	-6.638764
H	0.646895	0.888903	-5.879071

Table S15. Optimized Structure of $C_{\pi}(1)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
C	0.000000	0.000000	0.666694
C	0.000000	0.000000	-0.666694
H	0.931433	0.000000	1.240483
H	-0.931433	0.000000	1.240483
H	0.931433	0.000000	-1.240483
H	-0.931433	0.000000	-1.240483

Table S16. Optimized Structure of $C_{\pi}(2)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
C	0.000000	0.000000	1.854720
C	-0.436062	0.000000	0.584572
C	0.436062	0.000000	-0.584572
C	0.000000	0.000000	-1.854720
H	1.069090	0.000000	2.088662
H	-0.694200	0.000000	2.697693
H	-1.514669	0.000000	0.385740
H	1.514669	0.000000	-0.385740
H	-1.069090	0.000000	-2.088662
H	0.694200	0.000000	-2.697693

Table S17. Optimized Structure of $C_{\pi}(3)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
C	0.000000	0.000000	3.085075

C	-0.520423	0.000000	1.844357
C	0.264210	0.000000	0.623618
C	-0.264210	0.000000	-0.623618
C	0.520423	0.000000	-1.844357
C	0.000000	0.000000	-3.085075
H	1.081960	0.000000	3.247936
H	-0.637498	0.000000	3.971371
H	-1.610263	0.000000	1.722107
H	1.355426	0.000000	0.737393
H	-1.355426	0.000000	-0.737393
H	1.610263	0.000000	-1.722107
H	-1.081960	0.000000	-3.247936
H	0.637498	0.000000	-3.971371

Table S18. Optimized Structure of $C_{\pi}(4)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
C	0.000000	0.000000	4.320849
C	-0.553984	0.000000	3.093478
C	0.195318	0.000000	1.853342
C	-0.370417	0.000000	0.618715
C	0.370417	0.000000	-0.618715
C	-0.195318	0.000000	-1.853342
C	0.553984	0.000000	-3.093478
C	0.000000	0.000000	-4.320849
H	1.085934	0.000000	4.454236
H	-0.613842	0.000000	5.223685

H	-1.646938	0.000000	3.001446
H	1.289360	0.000000	1.934837
H	-1.464866	0.000000	0.541268
H	1.464866	0.000000	-0.541268
H	-1.289360	0.000000	-1.934837
H	1.646938	0.000000	-3.001446
H	-1.085934	0.000000	-4.454236
H	0.613842	0.000000	-5.223685

Table S19. Optimized Structure of $C_{\pi}(5)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
C	0.000000	0.000000	-5.557820
C	-0.571187	0.000000	-4.337881
C	0.159787	0.000000	-3.087955
C	-0.425204	0.000000	-1.860652
C	0.294456	0.000000	-0.614088
C	-0.294456	0.000000	0.614088
C	0.425204	0.000000	1.860652
C	-0.159787	0.000000	3.087955
C	0.571187	0.000000	4.337881
C	0.000000	0.000000	5.557820
H	1.087553	0.000000	-5.676214
H	-0.601165	0.000000	-6.468934
H	-1.665221	0.000000	-4.261658
H	1.254732	0.000000	-3.152608
H	-1.520652	0.000000	-1.801014

H	1.389811	0.000000	-0.671754
H	-1.389811	0.000000	0.671754
H	1.520652	0.000000	1.801014
H	-1.254732	0.000000	3.152608
H	1.665221	0.000000	4.261658
H	-1.087553	0.000000	5.676214
H	0.601165	0.000000	6.468934

Table S20. Optimized Structure of Si_{σ}(1) Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
Si	0.000000	0.000000	1.180789
Si	0.000000	0.000000	-1.180789
H	0.000000	1.404340	1.701154
H	1.216194	-0.702170	1.701154
H	-1.216194	-0.702170	1.701154
H	1.216194	0.702170	-1.701154
H	-1.216194	0.702170	-1.701154
H	0.000000	-1.404340	-1.701154

Table S21. Optimized Structure of Si_{σ}(2) Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
Si	0.855598	0.000000	0.818351
Si	-0.854267	-0.020862	-0.818051
Si	0.000000	0.000000	3.022635
Si	0.000000	0.000000	-3.022635

H	1.709474	1.218054	0.619465
H	1.731053	-1.203863	0.627158
H	-1.737075	1.176307	-0.618553
H	-1.700518	-1.245300	-0.626056
H	-0.85673	1.20853	3.24198
H	1.11437	0.01473	4.02382
H	-0.83307	-1.22317	3.25170
H	-1.11460	-0.02318	-4.02339
H	0.87125	-1.19685	-3.24868
H	0.81794	1.23444	-3.24563

Table S22. Optimized Structure of $Si_{\sigma}(3)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
Si	0.518618	0.000000	-1.063719
Si	-0.519609	0.000893	1.063842
Si	1.041894	-0.000758	2.843019
Si	-1.042435	0.000853	-2.843272
Si	0.000000	0.000000	4.966067
Si	0.000000	0.000000	-4.966067
H	1.399257	1.209626	-1.179935
H	1.397619	-1.210838	-1.179719
H	-1.39828	1.21194	1.18011
H	-1.40055	-1.20851	1.18002
H	1.91831	-1.21278	2.72176
H	1.92066	1.20960	2.72210
H	-1.92081	-1.20979	-2.72244

H	-1.91931	1.21261	-2.72267
H	1.02442	-0.00251	6.05930
H	-0.85886	1.21734	5.11750
H	-0.86343	-1.21426	5.11620
H	-1.02427	0.00000	-6.05945
H	0.86150	1.21552	-5.11705
H	0.86083	-1.21608	-5.11641

Table S23. Optimized Structure of $Si_{\sigma}(4)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
Si	0.745257	0.000000	0.919126
Si	-0.747072	0.000210	-0.919304
Si	0.371368	0.000396	-3.006264
Si	-0.372895	0.000414	3.006242
Si	1.121193	-0.000889	4.842585
Si	-1.122121	-0.000343	-4.843090
Si	0.000000	0.000000	6.924866
Si	0.000000	0.000000	-6.924866
H	1.628306	1.210332	0.835147
H	1.627705	-1.210774	0.835201
H	-1.629822	1.210762	-0.835356
H	-1.629828	-1.210345	-0.835476
H	1.255410	-1.209495	-3.089041
H	1.254524	1.210924	-3.089201
H	-1.257313	-1.209190	3.089130
H	-1.255606	1.211243	3.089460

H	2.003758	1.209505	4.754206
H	2.001641	-1.212824	4.754193
H	-2.004203	1.210434	-4.755167
H	-2.003133	-1.211886	-4.754959
H	-0.865228	1.216529	7.042740
H	0.982013	-0.000977	8.056325
H	-0.867397	-1.215010	7.042519
H	-0.981473	-0.000738	-8.056793
H	0.867086	-1.215274	-7.042041
H	0.865651	1.216264	-7.042384

Table S24. Optimized Structure of $Si_{\sigma}(5)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
Si	0.000000	0.000000	8.889515
Si	1.164725	0.000000	6.831275
Si	-0.290913	-0.011737	4.964298
Si	0.870715	-0.021069	2.901063
Si	-0.582426	-0.004982	1.031399
Si	0.580344	-0.031727	-1.031496
Si	-0.871898	0.018668	-2.901252
Si	0.289191	-0.025309	-4.964341
Si	-1.164048	0.053196	-6.831580
Si	0.000000	0.000000	-8.889515
H	-0.879684	1.208310	8.982563
H	-0.857511	-1.223105	8.995144
H	0.957669	0.014660	10.041552

H	2.041331	1.215689	6.757531
H	2.054363	-1.206622	6.764838
H	-1.174633	-1.222634	5.034565
H	-1.177345	1.197815	5.023293
H	1.766023	1.181385	2.835772
H	1.743981	-1.239610	2.835487
H	-1.486702	-1.200498	1.100123
H	-1.446543	1.220278	1.092966
H	1.499702	1.152646	-1.093142
H	1.428899	-1.267422	-1.100084
H	-1.800079	-1.158582	-2.835712
H	-1.711174	1.260885	-2.836089
H	1.230161	1.142326	-5.023223
H	1.116481	-1.275445	-5.034486
H	-2.108047	-1.111406	-6.765464
H	-1.984052	1.307767	-6.757920
H	-0.955631	0.058928	-10.041830
H	0.934392	1.166563	-8.982066
H	0.800341	-1.261257	-8.995124

Table S25. Optimized Structure of Si_{π}(1) Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
Si	0.000000	0.000000	1.089240
Si	0.000000	0.000000	-1.089240
H	1.310055	0.000000	1.806603
H	-1.030347	0.809092	1.806603

H	1.030347	-0.809092	-1.806603
H	-1.310055	0.000000	-1.806603

Table S26. Optimized Structure of $Si_{\pi}(2)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
Si	0.751140	0.000000	-0.873361
Si	-0.751210	-0.000175	0.873372
Si	0.000000	0.000000	2.934840
Si	0.000000	0.000000	-2.934840
H	1.945389	-0.868812	-0.624453
H	-1.945574	0.868533	0.624649
H	1.172566	-0.863899	3.267432
H	-0.967674	0.082830	4.070940
H	-1.172552	0.863960	-3.267309
H	0.967710	-0.082782	-4.070918

Table S27. Optimized Structure of $Si_{\pi}(3)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
Si	0.906780	0.000000	2.866972
Si	-0.448926	0.019394	1.010751
Si	0.449902	-0.019902	-1.010664
Si	0.000000	0.000000	4.867288
Si	-0.906096	-0.000262	-2.866662
Si	0.000000	0.000000	-4.867288

H	2.133831	0.845567	2.719524
H	-1.679455	-0.818868	1.177693
H	1.680406	0.818372	-1.177712
H	-1.210982	-0.841807	5.10355
H	-2.133252	-0.845616	-2.718902
H	1.210897	0.841823	-5.103803
H	-0.876721	-0.067712	-6.075774
H	0.876133	0.067965	6.076182

Table S28. Optimized Structure of Si_{π}(4) Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
Si	0.642568	0.000000	0.948292
Si	-0.643096	0.000436	-0.948246
Si	0.321218	-0.018937	-2.943270
Si	-0.321557	0.019445	2.943374
Si	0.970599	0.010695	4.841650
Si	-0.970679	-0.010238	-4.841706
Si	0.000000	0.000000	6.813079
Si	0.000000	0.000000	-6.813079
H	1.873609	0.845171	0.828991
H	-1.874062	-0.844882	-0.829126
H	1.551179	0.827459	-3.065694
H	-1.551185	-0.827417	3.065902
H	2.195886	0.864794	4.735147
H	-2.196303	-0.863856	-4.735255
H	-1.211266	-0.851845	7.008290

H	0.837677	0.070522	8.048783
H	1.211669	0.851247	-7.008324
H	-0.837585	-0.070409	-8.048845

Table S29. Optimized Structure of $Si_{\pi}(5)$ Calculated Using the RB3LYP/cc-pVDZ Method

Atom	*x*/Å	*y*/Å	*z*/Å
Si	0.502559	0.000000	0.990633
Si	-0.498402	-0.001308	-0.990630
Si	0.748358	0.016758	-2.908980
Si	-0.744808	-0.017886	2.908575
Si	-0.252648	0.022689	-4.887719
Si	1.005281	0.024676	-6.807776
Si	0.255225	-0.023623	4.887821
Si	0.000000	0.000000	-8.762243
Si	-1.003968	-0.025169	6.807078
Si	0.000000	0.000000	8.762243
H	1.726627	0.858122	1.083904
H	-1.722403	-0.859543	-1.083751
H	1.971878	0.875611	-2.813515
H	-1.968321	-0.876694	2.812554
H	-1.474366	-0.838659	-4.985904
H	2.222962	0.892106	-6.724561
H	1.476871	0.837784	4.986405
H	-1.205072	-0.865450	-8.934485
H	0.815521	0.076888	-10.012282
H	-2.22141	-0.892889	6.723288

H	1.204796	0.865703	8.935235
H	-0.816424	-0.076769	10.011709