

Si₇₈ double cage structure and special optical property

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Table S1. Wavelengths (nm), excitation energies, and oscillator strengths for 30 calculated excitations of $\text{Si}_{18}@\text{Si}_{60}$ and $\text{Si}_{18}@\text{Si}_{60}\text{H}_{52}$.

$\text{Si}_{18}@\text{Si}_{60}$				$\text{Si}_{18}@\text{Si}_{60}\text{H}_{52}$			
Electronic transitions	λ_{em} (nm)	f	Excitation energies (eV)	Electronic transitions	λ_{em} (nm)	f	Excitation energies (eV)
$S_0 \rightarrow S_1$	1848.0	0.0016	0.67	$S_0 \rightarrow S_1$	2944.9	0.0027	0.42
$S_0 \rightarrow S_2$	1541.0	0.0001	0.81	$S_0 \rightarrow S_2$	1423.2	0.0130	0.87
$S_0 \rightarrow S_3$	1521.1	0.0004	0.82	$S_0 \rightarrow S_3$	1218.9	0.0073	1.02
$S_0 \rightarrow S_4$	1399.0	0.0007	0.89	$S_0 \rightarrow S_4$	1014.1	0.0005	1.22
$S_0 \rightarrow S_5$	1362.9	0.0001	0.91	$S_0 \rightarrow S_5$	951.6	0.0046	1.30
$S_0 \rightarrow S_6$	1310.3	0.0005	0.95	$S_0 \rightarrow S_6$	926.9	0.0074	1.34
$S_0 \rightarrow S_7$	1243.7	0.0003	1.00	$S_0 \rightarrow S_7$	926.3	0.0007	1.34
$S_0 \rightarrow S_8$	1231.0	0.0008	1.01	$S_0 \rightarrow S_8$	815.8	0.0069	1.52
$S_0 \rightarrow S_9$	1220.3	0.0008	1.02	$S_0 \rightarrow S_9$	798.4	0.0046	1.55
$S_0 \rightarrow S_{10}$	1191.4	0.0022	1.04	$S_0 \rightarrow S_{10}$	734.6	0.0087	1.69
$S_0 \rightarrow S_{11}$	1157.1	0.0020	1.07	$S_0 \rightarrow S_{11}$	729.4	0.0017	1.70
$S_0 \rightarrow S_{12}$	1121.1	0.0030	1.11	$S_0 \rightarrow S_{12}$	712.1	0.0191	1.74
$S_0 \rightarrow S_{13}$	1108.1	0.0004	1.12	$S_0 \rightarrow S_{13}$	696.3	0.0019	1.78
$S_0 \rightarrow S_{14}$	1102.5	0.0021	1.13	$S_0 \rightarrow S_{14}$	691.1	0.0006	1.79
$S_0 \rightarrow S_{15}$	1085.1	0.0063	1.14	$S_0 \rightarrow S_{15}$	672.0	0.0005	1.85
$S_0 \rightarrow S_{16}$	1071.0	0.0015	1.16	$S_0 \rightarrow S_{16}$	663.5	0.0132	1.87
$S_0 \rightarrow S_{17}$	1069.3	0.0014	1.16	$S_0 \rightarrow S_{17}$	657.8	0.0016	1.88
$S_0 \rightarrow S_{18}$	1044.2	0.0017	1.19	$S_0 \rightarrow S_{18}$	648.5	0.0037	1.91
$S_0 \rightarrow S_{19}$	1035.1	0.0023	1.20	$S_0 \rightarrow S_{19}$	643.9	0.0012	1.92
$S_0 \rightarrow S_{20}$	1030.9	0.0020	1.20	$S_0 \rightarrow S_{20}$	643.0	0.0086	1.93
$S_0 \rightarrow S_{21}$	1009.6	0.0014	1.23	$S_0 \rightarrow S_{21}$	627.0	0.0016	1.98
$S_0 \rightarrow S_{22}$	1000.8	0.0020	1.24	$S_0 \rightarrow S_{22}$	610.9	0.0002	2.03
$S_0 \rightarrow S_{23}$	992.7	0.0001	1.25	$S_0 \rightarrow S_{23}$	608.3	0.0070	2.04
$S_0 \rightarrow S_{24}$	981.9	0.0008	1.26	$S_0 \rightarrow S_{24}$	603.8	0.0002	2.05
$S_0 \rightarrow S_{25}$	979.4	0.0004	1.27	$S_0 \rightarrow S_{25}$	591.5	0.0057	2.10
$S_0 \rightarrow S_{26}$	972.3	0.0048	1.28	$S_0 \rightarrow S_{26}$	588.7	0.0076	2.11
$S_0 \rightarrow S_{27}$	962.7	0.0003	1.29	$S_0 \rightarrow S_{27}$	582.1	0.0014	2.13
$S_0 \rightarrow S_{28}$	955.7	0.0007	1.30	$S_0 \rightarrow S_{28}$	574.7	0.0041	2.16
$S_0 \rightarrow S_{29}$	953.5	0.0022	1.30	$S_0 \rightarrow S_{29}$	570.8	0.0012	2.17
$S_0 \rightarrow S_{30}$	947.8	0.0007	1.31	$S_0 \rightarrow S_{30}$	565.1	0.0003	2.19

Table S2. Wavelengths (nm), excitation energies, and oscillator strengths for 30 calculated excitations of Si₁₄@Si₆₄ and Si₁₄@Si₆₄H₅₂.

Si ₁₄ @Si ₆₄				Si ₁₄ @Si ₆₄ H ₅₂			
Electronic transitions	λ_{em} (nm)	f	Excitation energies (eV)	Electronic transitions	λ_{em} (nm)	f	Excitation energies (eV)
S ₀ →S ₁	4062.2	0.0052	0.31	S ₀ →S ₁	1745.2	0.0140	0.71
S ₀ →S ₂	2552.6	0.0002	0.49	S ₀ →S ₂	1554.5	0.0013	0.80
S ₀ →S ₃	2098.4	0.0007	0.59	S ₀ →S ₃	1108.8	0.0032	1.12
S ₀ →S ₄	1931.7	0.0013	0.64	S ₀ →S ₄	1000.2	0.0047	1.24
S ₀ →S ₅	1807.3	0.0007	0.69	S ₀ →S ₅	960.4	0.0002	1.29
S ₀ →S ₆	1732.3	0.0023	0.72	S ₀ →S ₆	903.1	0.0024	1.37
S ₀ →S ₇	1623.7	0.0012	0.76	S ₀ →S ₇	857.3	0.0057	1.45
S ₀ →S ₈	1528.0	0.0013	0.81	S ₀ →S ₈	785.5	0.0016	1.58
S ₀ →S ₉	1429.4	0.0008	0.87	S ₀ →S ₉	773.0	0.0018	1.60
S ₀ →S ₁₀	1405.9	0.0019	0.88	S ₀ →S ₁₀	681.7	0.0047	1.82
S ₀ →S ₁₁	1338.9	0.0001	0.93	S ₀ →S ₁₁	666.7	0.0010	1.86
S ₀ →S ₁₂	1276.2	0.0007	0.97	S ₀ →S ₁₂	660.4	0.0060	1.88
S ₀ →S ₁₃	1248.7	0.0002	0.99	S ₀ →S ₁₃	656.5	0.0031	1.89
S ₀ →S ₁₄	1240.9	0.0011	1.00	S ₀ →S ₁₄	642.0	0.0015	1.93
S ₀ →S ₁₅	1233.8	0.0025	1.01	S ₀ →S ₁₅	622.6	0.0036	1.99
S ₀ →S ₁₆	1211.6	0.0038	1.02	S ₀ →S ₁₆	612.2	0.0010	2.03
S ₀ →S ₁₇	1184.6	0.0007	1.05	S ₀ →S ₁₇	601.5	0.0018	2.06
S ₀ →S ₁₈	1145.7	0.0026	1.08	S ₀ →S ₁₈	594.7	0.0034	2.08
S ₀ →S ₁₉	1135.4	0.0003	1.09	S ₀ →S ₁₉	582.1	0.0037	2.13
S ₀ →S ₂₀	1112.4	0.0047	1.11	S ₀ →S ₂₀	580.1	0.0004	2.14
S ₀ →S ₂₁	1106.0	0.0016	1.12	S ₀ →S ₂₁	577.1	0.0022	2.15
S ₀ →S ₂₂	1083.4	0.0003	1.14	S ₀ →S ₂₂	563.4	0.0003	2.2
S ₀ →S ₂₃	1076.2	0.0012	1.15	S ₀ →S ₂₃	551.9	0.0007	2.2
S ₀ →S ₂₄	1073.3	0.0009	1.16	S ₀ →S ₂₄	549.4	0.0001	2.26
S ₀ →S ₂₅	1056.5	0.0028	1.18	S ₀ →S ₂₅	547.7	0.0008	2.26
S ₀ →S ₂₆	1038.9	0.0037	1.19	S ₀ →S ₂₆	546.0	0.0012	2.27
S ₀ →S ₂₇	1025.2	0.0002	1.21	S ₀ →S ₂₇	544.6	0.0013	2.28
S ₀ →S ₂₈	1014.9	0.0012	1.22	S ₀ →S ₂₈	535.8	0.0008	2.31
S ₀ →S ₂₉	1012.4	0.0020	1.22	S ₀ →S ₂₉	533.2	0.0007	2.32
S ₀ →S ₃₀	995.8	0.0009	1.25	S ₀ →S ₃₀	532.2	0.0033	2.33

Table S3. Wavelengths (nm), excitation energies, and oscillator strengths of 30 calculated excitations of Diamod-like Si₇₈ and Diamond-like Si₇₈H₅₂.

Diamod-like Si ₇₈				Diamond-like Si ₇₈ H ₅₂			
Electronic transitions	λ_{em} (nm)	f	Excitation energies (eV)	Electronic transitions	λ_{em} (nm)	f	Excitation energies (eV)
S ₀ →S ₁	1955.1	0.0002	0.63	S ₀ →S ₁	367.3	0.0001	3.38
S ₀ →S ₂	1911.4	0.0009	0.65	S ₀ →S ₂	367.2	0.0000	3.38
S ₀ →S ₃	1908.3	0.0009	0.65	S ₀ →S ₃	367.1	0.0001	3.38
S ₀ →S ₄	1706.9	0.0041	0.73	S ₀ →S ₄	366.4	0.0090	3.38
S ₀ →S ₅	1699.4	0.0041	0.73	S ₀ →S ₅	366.3	0.0091	3.38
S ₀ →S ₆	1602.5	0.0051	0.77	S ₀ →S ₆	366.2	0.0090	3.39
S ₀ →S ₇	1344.6	0.0000	0.92	S ₀ →S ₇	365.7	0.0001	3.39
S ₀ →S ₈	1313.5	0.0001	0.94	S ₀ →S ₈	365.6	0.0000	3.39
S ₀ →S ₉	1312.7	0.0001	0.94	S ₀ →S ₉	364.8	0.0000	3.40
S ₀ →S ₁₀	1312.4	0.0003	0.94	S ₀ →S ₁₀	364.5	0.0000	3.40
S ₀ →S ₁₁	1311.1	0.0003	0.95	S ₀ →S ₁₁	364.0	0.0001	3.41
S ₀ →S ₁₂	1305.5	0.0002	0.95	S ₀ →S ₁₂	363.9	0.0000	3.41
S ₀ →S ₁₃	1293.0	0.0000	0.96	S ₀ →S ₁₃	363.8	0.0000	3.41
S ₀ →S ₁₄	1273.2	0.0002	0.97	S ₀ →S ₁₄	363.7	0.0001	3.41
S ₀ →S ₁₅	1272.1	0.0002	0.97	S ₀ →S ₁₅	363.6	0.0001	3.41
S ₀ →S ₁₆	1268.0	0.0022	0.98	S ₀ →S ₁₆	363.6	0.0001	3.41
S ₀ →S ₁₇	1180.6	0.0006	1.05	S ₀ →S ₁₇	363.5	0.0001	3.41
S ₀ →S ₁₈	1180.1	0.0004	1.05	S ₀ →S ₁₈	363.5	0.0002	3.41
S ₀ →S ₁₉	1178.7	0.0002	1.05	S ₀ →S ₁₉	345.2	0.0000	3.59
S ₀ →S ₂₀	1177.8	0.0000	1.05	S ₀ →S ₂₀	345.2	0.0000	3.59
S ₀ →S ₂₁	1162.7	0.0000	1.07	S ₀ →S ₂₁	345.2	0.0000	3.59
S ₀ →S ₂₂	1162.2	0.0000	1.07	S ₀ →S ₂₂	341.9	0.0001	3.63
S ₀ →S ₂₃	1158.6	0.0001	1.07	S ₀ →S ₂₃	341.6	0.0001	3.63
S ₀ →S ₂₄	1156.8	0.0001	1.07	S ₀ →S ₂₄	341.5	0.0001	3.63
S ₀ →S ₂₅	1154.3	0.0070	1.07	S ₀ →S ₂₅	331.5	0.0000	3.74
S ₀ →S ₂₆	1141.4	0.0008	1.09	S ₀ →S ₂₆	331.5	0.0000	3.74
S ₀ →S ₂₇	1139.7	0.0002	1.09	S ₀ →S ₂₇	331.5	0.0000	3.74
S ₀ →S ₂₈	1139.2	0.0003	1.09	S ₀ →S ₂₈	329.6	0.0000	3.76
S ₀ →S ₂₉	1135.7	0.0007	1.09	S ₀ →S ₂₉	329.6	0.0000	3.76
S ₀ →S ₃₀	1135.1	0.0006	1.09	S ₀ →S ₃₀	329.5	0.000	3.76

The coordinates of Si₇₈ isomers :

(a) Si₁₈@Si₆₀:

Si	1. 69489000	-5. 09035400	1. 10212700
Si	3. 64778000	-4. 52675600	2. 44618700
Si	2. 67468000	-2. 78335100	3. 67511400
Si	3. 61311000	-0. 95205100	4. 76799200
Si	1. 61118900	0. 31644400	5. 06939400
Si	1. 54154300	2. 68169200	5. 01964100
Si	2. 83585200	3. 40312300	3. 18393300
Si	4. 55015800	0. 40330700	3. 00573500
Si	5. 00864400	2. 44353600	0. 52546800
Si	6. 28165500	0. 64675700	-0. 49580000
Si	5. 42661600	-0. 86478900	1. 13189500
Si	4. 69630400	-3. 05353900	0. 77579500
Si	4. 57978800	-3. 96598700	-1. 48479800
Si	4. 16141300	-2. 10447800	-2. 90958300
Si	-1. 80334700	-0. 35198600	-5. 56775800
Si	2. 34334100	-4. 83833900	-1. 08824900
Si	-3. 35318200	0. 87116100	-4. 13384600
Si	-5. 49357200	-0. 18408200	-3. 49136900
Si	-0. 51773900	-5. 92942600	1. 73978200
Si	-1. 99489300	-5. 03970200	0. 11852300
Si	-3. 79788200	-3. 82096800	1. 03717800
Si	-1. 20733200	-4. 15992000	3. 18114600
Si	-3. 57281200	-3. 73718000	3. 45228100
Si	-5. 68319500	0. 96092600	-1. 28813100
Si	-3. 64661100	-1. 39036200	3. 85136500
Si	0. 40515700	-3. 00742900	4. 32897100
Si	-0. 32762400	-0. 89182200	5. 12847000
Si	-2. 58538400	1. 89292400	4. 45550200
Si	-0. 64496900	3. 20586700	4. 28950500
Si	0. 43646300	5. 08508500	-1. 63225900
Si	5. 16915100	2. 78722300	2. 93523000
Si	-1. 81177600	-5. 44606300	-2. 18564500
Si	0. 44236900	-4. 71830600	-2. 55022600
Si	0. 86068700	-3. 20210100	-4. 22031500
Si	3. 00644100	-2. 33176500	-5. 03637900
Si	5. 14177600	0. 03491200	-2. 61239700
Si	-0. 40287600	2. 91407700	-4. 32924000
Si	1. 33467200	4. 54928300	-3. 80839400
Si	-2. 85921500	3. 25482100	-4. 45124700
Si	2. 05064500	5. 02087400	0. 01385400
Si	1. 87233400	5. 39138000	2. 31975300
Si	-1. 88356500	5. 72770300	-1. 21361800

Si	-3.04249300	3.89668500	-2.19733400
Si	-0.47227600	4.88425700	2.66628400
Si	-3.86706700	3.35178900	1.34208500
Si	-2.57285000	-0.23402800	5.64319400
Si	-4.76250400	2.49564400	3.43386800
Si	-5.10446700	0.11412500	2.75627100
Si	-5.55765300	-0.55856700	0.50445600
Si	-2.84321000	-3.47043800	-3.14714000
Si	-4.54707800	-2.11215000	-2.31582100
Si	-1.34331000	-2.36364100	-4.60561900
Si	-5.60156300	-2.83026300	-0.28256500
Si	2.35830700	0.00567600	-4.87021500
Si	0.20642800	0.83257500	-5.28684900
Si	-4.90387200	3.19794000	-0.78604200
Si	4.23589400	1.53013200	-4.35258400
Si	3.06600000	3.12924700	-3.05360300
Si	3.92867300	3.89314800	-0.95689600
Si	-2.24907500	5.03184200	1.08320900
Si	1.24600700	-0.14657100	-2.77809800
Si	3.11130600	-0.00431600	-1.45242800
Si	2.61096100	1.85992700	-0.10731900
Si	0.53477600	2.89540300	-0.56446600
Si	-0.19036000	1.61468700	-2.37509100
Si	0.28967800	-2.14968900	-2.01976000
Si	1.26308400	-2.84002400	0.07151500
Si	2.98416300	-1.36690100	0.41416800
Si	-1.97210300	-1.72650700	-1.64034300
Si	-2.25302900	-2.09418600	0.65543000
Si	-0.19331800	-2.25450500	1.83471500
Si	-3.05496500	-0.05953600	1.50244800
Si	-3.46061100	1.25744300	-0.39905000
Si	-2.18681900	0.51920700	-2.16747400
Si	-1.39844600	1.23702600	2.52649600
Si	0.39056700	-0.16600900	2.80046100
Si	-0.93542400	3.02621900	1.20022400
Si	2.48596200	0.40401800	1.86828200

(b) Si₁₆@Si₆₂:

Si	-3.22063200	-3.48599100	2.53173600
Si	-5.57119400	-3.33894700	1.78039500
Si	-2.65747900	-3.06565800	4.98736400
Si	-3.56354800	-0.95785500	4.36389600
Si	-5.22290600	-1.22013500	2.72122200
Si	-5.16943200	0.75370100	1.48214700

Si	-3.75740200	2.19240900	2.68205500
Si	-2.87243200	1.18245100	4.63570600
Si	-0.50048400	1.67351500	4.79760500
Si	0.93638700	-0.17230800	5.51911300
Si	-0.36216400	-2.13508900	4.69270500
Si	1.05263200	-3.74764700	3.67855800
Si	0.25853700	-5.44016200	2.20696800
Si	-1.73660700	-4.72406200	1.17406000
Si	2.04746800	-5.20326000	0.67631900
Si	4.20016700	-4.81584100	1.63305000
Si	3.25870200	-3.26377600	3.20047400
Si	4.86978400	-3.04382900	0.27148400
Si	4.68010600	-1.46376900	4.01857300
Si	5.18325400	-1.04720000	1.59988000
Si	2.83254300	0.06892400	4.17173800
Si	5.31520400	0.98915400	0.45312300
Si	5.31367600	2.84302000	1.96465900
Si	3.29485500	2.21833300	3.15718400
Si	1.84541200	4.01420900	3.54749400
Si	2.48727800	5.63379600	2.02843300
Si	3.94942100	4.28994300	0.72414500
Si	-0.13178800	4.09263000	4.82375400
Si	-1.06347800	4.55386300	2.60571200
Si	-3.36967000	4.38143700	1.89237700
Si	0.39169600	5.57349800	1.05477800
Si	-4.00572300	1.58480000	-3.31299700
Si	-1.94572200	1.91070000	-4.44656800
Si	-1.25174000	4.08048400	-4.08193200
Si	-1.74740100	4.79137500	-1.82023400
Si	-3.56584900	4.09763800	-0.58980200
Si	-5.33972600	3.10251700	-1.89093700
Si	-5.87883500	1.12326000	-0.72419700
Si	-6.67023100	-0.87477000	-1.73946100
Si	-5.15445000	-2.29529500	-0.41598600
Si	-4.86320500	-0.57555600	-3.20962300
Si	-3.64848600	-2.35653400	-4.06557600
Si	-3.70158700	-3.33266100	-1.96760000
Si	-1.91037000	-4.65790700	-1.26058900
Si	-0.38031200	-5.56453800	-2.92411000
Si	0.11027200	-3.49775800	-4.03896800
Si	-1.36022700	-1.65095800	-4.42644300
Si	-0.69590900	0.31989600	-5.75396900
Si	1.42617800	0.75452500	-4.51559100
Si	2.81675600	2.71331800	-4.79831300

Si	1. 03474600	3. 81194000	-3. 77264900
Si	1. 58648800	4. 68470200	-1. 69752300
Si	3. 94849000	4. 73372500	-1. 54341000
Si	-0. 04879700	6. 32028700	-1. 09242500
Si	3. 97367900	2. 65514500	-2. 64150400
Si	5. 45519600	1. 02348600	-1. 92103500
Si	2. 87218500	-1. 14014900	-4. 24570200
Si	4. 58596100	-1. 07172900	-2. 64756500
Si	5. 40162300	-3. 25054700	-2. 02123800
Si	3. 30869100	-4. 08242600	-2. 71532500
Si	1. 63137000	-5. 25028700	-1. 58950300
Si	2. 35066900	-3. 34385300	-4. 70947900
Si	1. 79536100	1. 65686900	1. 33528000
Si	0. 93444700	2. 46992200	-0. 83274600
Si	3. 00743800	-0. 31100200	0. 76849600
Si	2. 56911600	-1. 05394900	-1. 37840000
Si	1. 03672200	0. 48792500	-2. 19193500
Si	-1. 46608600	2. 55980800	-0. 76523200
Si	-0. 12810500	1. 09122600	2. 58841500
Si	-1. 68042200	2. 47951500	1. 51449900
Si	-0. 26682800	-1. 20448900	2. 54419100
Si	-1. 99105300	-1. 86888900	1. 23785700
Si	1. 73002400	-2. 09700500	1. 66403600
Si	1. 38803500	-2. 97800800	-0. 53947900
Si	-0. 91062800	-2. 59269700	-0. 72290700
Si	-0. 90818600	-0. 82871000	-2. 25421000
Si	-2. 56699700	0. 66516700	-1. 61454800
Si	-3. 59447700	-0. 57386800	0. 15023000

(c) Si₁₄@Si₆₄:

Si	5. 18842100	2. 72540000	-0. 94629900
Si	3. 66900000	0. 40953400	3. 68222400
Si	6. 09530300	1. 00326700	-2. 32683700
Si	4. 07457400	0. 39405200	-3. 42514600
Si	5. 59916900	-2. 99111000	-2. 22710700
Si	3. 86127800	-1. 94279500	-3. 53550800
Si	4. 13318900	-4. 15576600	-0. 80267100
Si	2. 35449200	-2. 76404400	-5. 21178400
Si	1. 34781500	-3. 86555300	-3. 38770500
Si	0. 88802300	-0. 89720100	-5. 04680200
Si	-0. 98689900	-3. 63750700	-3. 23142200
Si	-1. 11898400	-1. 44797900	-4. 00283000
Si	-2. 75396300	-4. 89512600	1. 80133600
Si	-2. 56333100	-4. 94979900	-2. 21191300

Si	-4.15253500	-3.12466200	-2.04803800
Si	-5.10064700	-1.57483000	-3.68481900
Si	-5.67339900	-3.14978700	-0.26384300
Si	-7.32614100	-1.48200300	-0.25510200
Si	-6.12598300	-0.36576500	-1.91160900
Si	-5.46321800	-1.62445500	3.24389600
Si	-2.99770600	2.03134900	-4.28530500
Si	-1.50964700	-1.57995500	3.90180700
Si	-3.17060000	-0.24689300	-3.76856700
Si	-1.27287500	-3.75802300	3.13802300
Si	1.79638800	-2.87533400	5.44952700
Si	0.88460100	1.28715200	-5.89089800
Si	2.62536700	1.88336900	-4.43080800
Si	0.37549200	-1.00781300	5.11256000
Si	-0.54807100	2.25843200	-4.18780600
Si	0.33789200	4.18571100	-3.29011300
Si	2.62047400	4.10809200	-3.72582000
Si	3.46963100	4.11772600	-1.52598100
Si	2.77404300	5.71120200	0.10844000
Si	0.49843300	4.94947900	-0.03399000
Si	-0.80138200	5.68910100	-1.92493300
Si	-0.93427700	4.83981800	1.82728800
Si	-3.12337600	4.80082000	1.08603400
Si	-2.63781300	4.42187900	-1.14921200
Si	-4.30450400	2.93745400	2.00906200
Si	-6.49734000	2.18201900	1.17378700
Si	-5.67132300	1.76353600	-1.12629000
Si	-4.13299100	3.16926700	-2.45840800
Si	-6.29069700	-0.24583500	1.47893100
Si	-3.49233300	-0.31986200	3.41718500
Si	-3.32940200	1.97919600	3.91683600
Si	0.89139200	-5.18599600	0.00691400
Si	-0.90072400	2.33872400	3.98885400
Si	2.31337500	-5.20620900	-1.79990200
Si	-0.26137100	4.66514400	4.05912300
Si	1.96677700	3.88825300	3.71017600
Si	3.29293400	4.14750100	1.80642600
Si	5.03039800	2.71737800	1.41662800
Si	5.83492800	0.97728200	2.82073900
Si	2.23029600	1.90466300	4.71110000
Si	0.28195900	1.19831600	5.76156800
Si	3.56660400	-1.85066500	4.23257100
Si	4.34786800	-2.63268000	2.21030400
Si	5.48077300	-0.77277000	1.23478600

Si	5.79159500	-0.94974600	-1.01109800
Si	4.44588700	-4.85062100	1.44439100
Si	2.11784200	-5.11012900	1.91237100
Si	0.98122800	-4.08617000	3.57804400
Si	-4.32860500	-3.05869600	1.62651900
Si	-1.31773500	-4.45101600	-0.13676800
Si	0.08036500	-0.87715300	-1.93550000
Si	2.45394700	-0.88245000	-1.95837600
Si	3.30889700	-0.19241800	0.12309800
Si	2.34076600	-1.00160900	2.11328900
Si	-0.04660900	-1.02386400	1.96128100
Si	2.95608300	2.14049400	0.08304300
Si	-0.49733500	1.32326800	1.81810700
Si	-2.80568700	1.09124000	1.56705400
Si	-3.86439400	0.32665200	-0.37294900
Si	-3.27152000	-1.88565400	-0.20478500
Si	-0.89358000	-2.05732900	-0.05251900
Si	-0.22918000	1.47277100	-1.89250300
Si	0.61721800	2.51457800	0.06376500
Si	-2.52854100	1.42315000	-1.91512200

(d) Si₂₀@Si₅₈:

Si	-4.87021600	0.53688200	-2.87169800
Si	-4.47182300	-1.75750200	-3.23799300
Si	-2.73523400	-4.64798200	-1.50379800
Si	-1.95243800	-5.78304900	0.46656100
Si	0.43014100	-5.57499200	0.18395100
Si	1.48456300	-4.86448200	-1.78134300
Si	0.50507900	-4.73840100	-3.94429600
Si	-1.71425600	-3.94213300	-3.50431600
Si	-4.37035800	-2.98012200	-1.24971000
Si	-4.94561800	-2.33224500	0.91597700
Si	-5.20737300	0.00690300	1.02462300
Si	-3.84226600	2.14405000	-4.38657600
Si	-2.95818100	-2.50868100	-5.01424700
Si	1.94193700	6.14151000	-0.60443600
Si	4.28296400	2.91399400	1.23008100
Si	5.32106100	0.03312800	-1.12008900
Si	5.77968500	-1.41871800	0.77634800
Si	4.86845500	1.89616000	3.29341100
Si	2.70487700	2.34432900	4.30728400
Si	-3.31850300	3.50226600	-2.45518900
Si	-5.03319400	3.83145200	-0.80796400
Si	-5.59460100	1.43140200	-0.79637900

Si	-5.09513300	0.53928500	3.32261300
Si	-3.65530700	2.34875100	2.96344500
Si	-3.76840800	3.97441800	1.26280400
Si	-1.58732500	4.83491300	1.44619300
Si	-0.44529900	5.55089400	-0.48623400
Si	-1.51816200	4.98798400	-2.56461200
Si	0.39087400	4.33223500	-3.88169700
Si	-1.00449300	0.82893200	5.19093700
Si	-1.81238900	2.84992700	4.34803800
Si	-0.63582600	4.82022500	3.61790800
Si	1.50684000	3.99312500	3.11971900
Si	1.35966200	0.64993400	5.17677500
Si	-2.06854900	-1.20406000	5.75057300
Si	-3.56230800	-1.29340600	3.83803900
Si	-4.32059500	-3.43945700	2.97828200
Si	-2.17337000	-4.08185700	2.12261700
Si	-0.38192400	-4.30102200	3.64205400
Si	-0.12216300	-2.12935100	4.67114500
Si	2.00680500	-1.58357800	5.63777200
Si	3.32089600	-2.04197000	3.67255600
Si	3.67721400	-4.24279900	2.68105800
Si	1.42109100	-4.53471800	2.07406700
Si	3.83011800	-4.25452000	-1.61173800
Si	4.14697300	-3.25943400	0.54515600
Si	4.56131700	-0.36395900	2.58129100
Si	5.19847600	-0.68224200	-3.40210000
Si	3.52063200	-2.33876400	-3.01913700
Si	1.78294400	-2.79479500	-4.56934100
Si	0.77963000	-1.18226100	-5.98482900
Si	1.62662200	0.87335300	-5.14340100
Si	3.64503800	1.11121500	-3.93952700
Si	3.93239000	3.05750200	-2.58504300
Si	1.99761500	4.26164600	-2.10625600
Si	-0.26189900	2.40525900	-5.16551300
Si	5.47353900	2.46725100	-0.80351400
Si	2.76761000	4.75171600	1.28148200
Si	-1.89707000	-0.86209700	2.30250900
Si	-3.24144000	0.81859900	-0.81754300
Si	-1.02905700	1.28847600	2.63131400
Si	-2.16051700	2.23558300	0.73205300
Si	1.30717500	1.25406100	2.58310600
Si	-2.17631600	1.12695800	-2.98747400
Si	1.90901100	-0.95222400	2.15421800
Si	-0.09878900	-2.35457900	2.11449900

Si	-2.88325600	-1.22261700	0.19861400
Si	-1.62065100	-2.46532700	-1.35968900
Si	0.31207400	-3.17784400	-0.18139200
Si	2.34468300	-2.32239100	-0.93400900
Si	3.38911600	-0.65240300	0.34062200
Si	3.11954900	1.50195100	-0.74411700
Si	1.68039000	2.67224600	0.73465200
Si	-0.32369700	3.18707200	-0.40170800
Si	-0.04214100	2.30044900	-2.59869300
Si	1.71718000	0.75342100	-2.51639600
Si	0.58688800	-1.04512900	-3.41346700
Si	-1.73097200	-1.22834500	-3.41888200

(e) Diamond-like:

Si	1.33756000	-1.64469100	-5.28185400
Si	-0.93020500	-2.21516200	-5.85919900
Si	-0.94194500	-6.04992500	1.61821700
Si	1.33752200	1.11142200	-5.41854500
Si	-0.92970500	1.62356300	-6.05061400
Si	-1.61587900	-0.23032500	-4.64333800
Si	-0.94531300	-3.96571100	4.84662900
Si	1.50797200	3.51346000	-2.26592900
Si	-0.77013100	3.71070200	-2.39587300
Si	-0.78110800	0.21992400	4.40902800
Si	1.33054100	5.39725800	1.22012000
Si	-0.93768100	6.18130300	1.00972500
Si	-1.62404000	4.13498500	2.11847200
Si	1.32676300	4.13977900	3.67510400
Si	-0.94311200	4.42901300	4.42897400
Si	2.38933000	1.77993400	-3.43932200
Si	1.32638500	-5.25048000	1.74972400
Si	5.01923200	-4.11174300	2.66033000
Si	2.37916600	-1.75769200	3.45646500
Si	1.32411400	-3.75399900	4.06723600
Si	1.49749600	0.20736000	4.17652300
Si	2.38044800	2.09159400	3.26625700
Si	2.38579500	3.86905400	-0.20177300
Si	-4.03615000	-4.02620400	2.59499400
Si	-1.84501300	-1.74472700	5.07537600
Si	-4.08009400	-1.77737900	3.40660800
Si	-3.95936700	-0.95390500	5.56602200
Si	-1.84353000	2.24206400	4.87665700
Si	-4.01695000	0.10033400	1.99837200
Si	-5.27139700	0.00126300	-0.00734000

Si	-4.07733200	2.10913500	3.21233800
Si	-4.07538000	-3.84088000	0.21108200
Si	-4.01283500	-1.78473600	-0.92035000
Si	-4.06862000	-2.06503900	-3.25056800
Si	-4.01199300	1.68676900	-1.09372600
Si	-1.83789400	-5.34451400	-0.50149700
Si	-3.95057900	-5.47039900	-1.42768200
Si	-1.83278000	-3.52441800	-4.05196400
Si	4.62004200	-1.82411100	2.80642900
Si	4.62247200	-3.30372800	0.51461900
Si	5.93041300	0.10909500	2.23556600
Si	4.99653900	-0.00150200	0.00640000
Si	5.93493400	-1.98634500	-1.00940800
Si	4.62753400	-1.51453800	-2.97121800
Si	5.93645400	1.87232300	-1.20173400
Si	4.62903800	1.21137500	-3.10778900
Si	4.62521100	3.33513400	0.18411800
Si	-4.02455400	-0.23797600	-4.79266100
Si	-4.06894900	1.73417600	-3.44051500
Si	-1.83568600	5.27057800	-1.02929600
Si	-1.83053200	3.10548600	-4.38184900
Si	-4.07312700	3.84517100	-0.17195300
Si	-4.03327300	4.26661100	2.18171000
Si	4.62092300	2.08979200	2.61151400
Si	2.38334700	-3.87318300	0.18163000
Si	-1.62674300	-3.90336000	2.51871700
Si	-0.77157900	-3.92844500	-2.01576300
Si	1.50782300	-3.72603800	-1.90905000
Si	2.38780300	-2.11292200	-3.24466400
Si	5.03037300	-0.24379500	-4.87878300
Si	2.96686900	-0.31129900	-6.24752300
Si	-3.94778700	5.30397900	-1.96411000
Si	-3.94745800	-4.34697900	-3.61821500
Si	-3.95794200	1.50450800	5.44290300
Si	5.02469700	4.35160500	2.23952900
Si	2.95775400	5.56804400	2.85963300
Si	-3.94427000	3.96816300	-4.03198000
Si	2.95258300	-5.25937700	3.39927800
Si	-1.58817900	0.10613900	2.12701100
Si	-0.81086600	-1.96600700	1.26824200
Si	-0.80956700	2.08225900	1.06684100
Si	-1.58248200	1.79236600	-1.15837600
Si	1.57367300	1.91518900	0.98523900
Si	1.57242000	-1.81027200	1.16913200

Si	-1.58356300	-1.89609800	-0.97484700
Si	2.56104000	-0.00110800	0.00319700
Si	-0.80540400	-0.11550700	-2.33842400
Si	1.57672700	-0.10639000	-2.14823000

(f) Si₁₂@Si₆₆:

Si	0.15998700	-6.26970300	0.19271200
Si	-1.70539800	-5.20256900	-0.75154200
Si	-3.93229800	-5.16038600	-0.20006400
Si	-3.68712100	-3.90516700	1.72071200
Si	-1.95932700	-4.55743900	3.20728800
Si	0.03652600	-4.62884600	1.93052800
Si	1.73557700	-5.00081900	-0.98904200
Si	0.16406300	2.92893700	-3.10887600
Si	2.01285700	-4.01973700	-3.09357600
Si	0.13351500	-3.27619600	-4.08191800
Si	-1.49208400	-3.57832000	-2.39854400
Si	-3.62653100	-3.16707900	-3.20558200
Si	-5.29943900	-4.56312000	-2.20516000
Si	-5.55230100	-2.29375400	-1.77004500
Si	-5.19372100	-1.19490700	0.26645800
Si	-5.46956700	-2.43112000	2.31344200
Si	-4.23015900	-0.80840400	3.53612600
Si	-2.40458800	-0.97908600	4.90496700
Si	-1.14557500	-2.91327400	4.53857600
Si	-1.42466100	0.97406600	5.76665100
Si	1.12838400	-3.15664800	5.29817000
Si	2.07939100	-1.09887900	4.72445800
Si	0.46119700	0.50918800	4.38711300
Si	4.09566400	-0.50334900	3.80167100
Si	2.21062600	5.87931100	2.20872400
Si	1.87207000	-3.98983700	3.28083000
Si	3.85061000	-3.41860300	2.18170800
Si	5.72115000	-2.04237700	2.93290100
Si	1.49619600	5.53315500	-1.63434400
Si	3.70759300	-4.31468100	0.00733800
Si	4.90398900	-3.30823500	-1.70378900
Si	6.60515300	-1.85829100	-1.21382300
Si	5.81786000	-0.93932900	0.79276500
Si	5.54889600	-0.30833500	-2.62809700
Si	4.15199000	-3.56807700	-3.88822500
Si	-3.67213400	3.63120400	0.29503400
Si	-5.60014500	2.71441400	1.43855800
Si	-4.32316700	1.52198200	3.05084100

Si	-2.29712500	2.19361900	3.91533100
Si	-1.52063600	4.43977600	3.66057600
Si	-2.16649800	4.97669300	1.52828000
Si	-1.47853300	6.77043600	0.25400800
Si	0.74081100	6.25549200	0.45975700
Si	0.71108300	4.32689800	3.05181800
Si	1.58952000	2.18419500	3.18622700
Si	3.85431700	1.69367100	3.29849200
Si	5.21810800	2.97577400	1.90796000
Si	3.55459500	4.31484200	0.96861400
Si	5.32560300	1.26907600	0.26556800
Si	3.55708000	4.67627300	-1.31112500
Si	3.98725600	2.75157300	-2.53758500
Si	6.06353400	1.86305600	-1.96946500
Si	2.23868900	1.80301300	-3.73091200
Si	2.32487700	0.06021100	-5.48196900
Si	3.77953300	-1.17070900	-3.90260400
Si	0.25891700	-0.90075100	-4.45477700
Si	-1.80098600	-0.00769200	-5.35766400
Si	-1.88463100	1.81815400	-3.94275000
Si	-3.71133900	2.58839400	-2.72875400
Si	-5.36172200	-0.49577200	-3.19747400
Si	-5.91892600	1.63244100	-2.51075800
Si	-5.68025500	1.05709000	-0.21354300
Si	-3.89896500	4.77310500	-1.83036600
Si	-1.73349600	5.49734800	-1.72275600
Si	-0.03180700	5.34319300	-3.36015900
Si	-3.59355000	-1.21726800	-4.42736800
Si	-2.49806900	1.80829200	-0.75323800
Si	-0.16516900	1.74097400	-1.07425600
Si	-2.93127300	-0.40882000	-0.00974500
Si	-1.13140500	-1.82554100	-0.82890500
Si	0.20477200	-2.41627200	1.04650600
Si	-0.07047300	-0.38063000	2.22823900
Si	0.25851800	-0.40181200	-2.11204500
Si	3.12307900	0.07590000	0.13668200
Si	1.16131900	1.22335100	0.93408300
Si	2.51834300	-2.19484800	0.61502700
Si	2.58703400	-0.06153800	-2.12128400
Si	-2.35720800	0.13312400	2.21738800