Stable Thin Clathrate Layers

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Supplemental Material

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S1. Comparison of Column-XIV Bulk Energies

Config.	C	Si	Ge	Sn	Pb
fcc	4573	608	331	75	**-3.598**
bcc	4367	587	341	86	42
graphite	**-9.231**	640	602	570	719
hP1	971	352	243	45	96
tI4	cF8	328	228	46	128
cF8	131	**-5.420**	**-4.516**	**-3.863**	251
lonsdaleite	155	11	18	16	292
clathI	239	64	33	28	279
clathII	205	54	27	23	280
clathIII	260	81	48	40	288
clathIV	243	69	38	31	276*
deca	241	71	41	35	299*
icosa	288	92	59	49	274*
CFS-6	241	55	35	30	286
CFS-5	263	41	39	36	289
T12	238	45	36	32	278
amorph	–	158	128	91–101	–

Table S1.1: Bulk energies of famous Column-XIV allotropes, that were taken into slab internal-energy competition, see Section 4 in the main text. Internal energies of 17 bulk configurations of G4 elements after cell and atomic relaxations starting from sound initial atomic positions and lattice parameters. cF8 stands for the cubic diamond phase; lonsdaleite (wurtzite) is the hexagonal diamond polytype with eclipsed bond conformations. "deca" stands for "decagonal clathrate approximant", *Pearson symbol* oP392. "icosa" means "icosahedral clathrate approximant", cI920. „clathI" (cP46), "clathII" (cF136), "clathIII" (hP40) and "clathIV" (tP172) denotes type I, II, III and IV clathrate, respectively. "CFS" means Chiral Framework Structures (including T12), see Subsection 4.6 (of the main text). "amorph" denotes sp^3-amorphous phases of Ge and Si, visit Subsection 4.5; for Sn the lower bound corresponds to a-metal, whereas upper bound to an abstract a-sp^3 Sn obtained by a-Ge rescaling to the typical Sn interatomic distances. Kohn-Sham energies in eV/atom of the most stable (GS) structures are **highlighted by red**. GS energies have been subtracted from the remaining energies and the corresponding differences $E - E_{\mathrm{GS}}$ are stated in units of meV/atom for easier comparison of *distinct* elements. * – amorphized or strongly deformed during relaxation process. Without former annealing or external strain. Converged on K-points with default VASP DFT PAW GGA (PW91) ENCUT-s.

S2. Surface Reconstruction of Decagonal Tiles

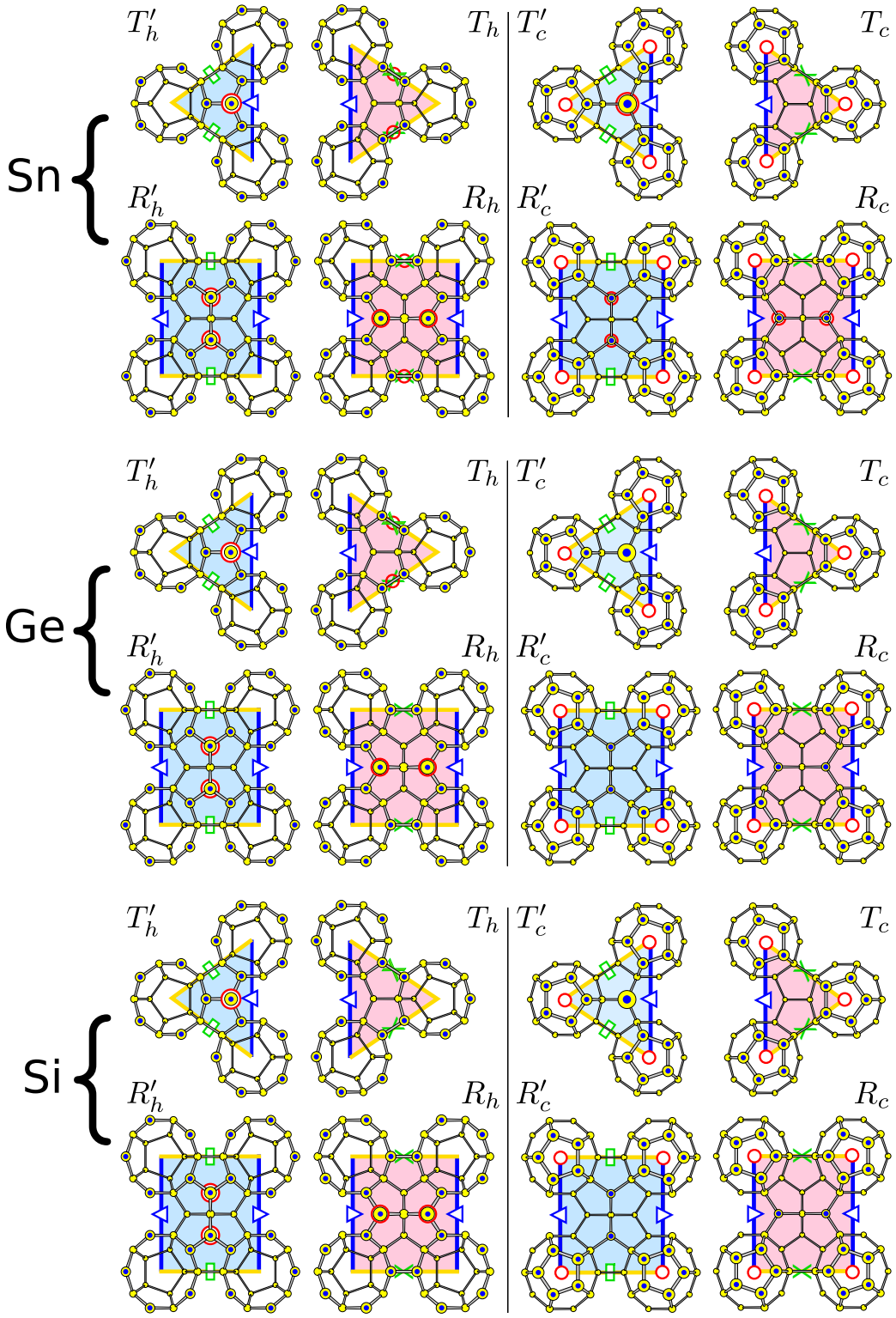

Figure S2.1: Reconstruction of *decagonal* Sn, Ge, Si clathrate tiles: isosceles triangle (T) and rectangle (R) terminated by cage "caps" (c) and "holes" (h). Adatoms (beneath the original atoms, inside the film) highlighted by red rings. 3-coord. atoms before the reconstruction marked with central blue dots, the rest are 4-coord. atoms. Side lengths distinguished by blue (longer) and yellow (shorter) color. Sides that fit together marked with green crosses, rectangles.

S3. Surface Reconstruction of Dodecagonal Tiles

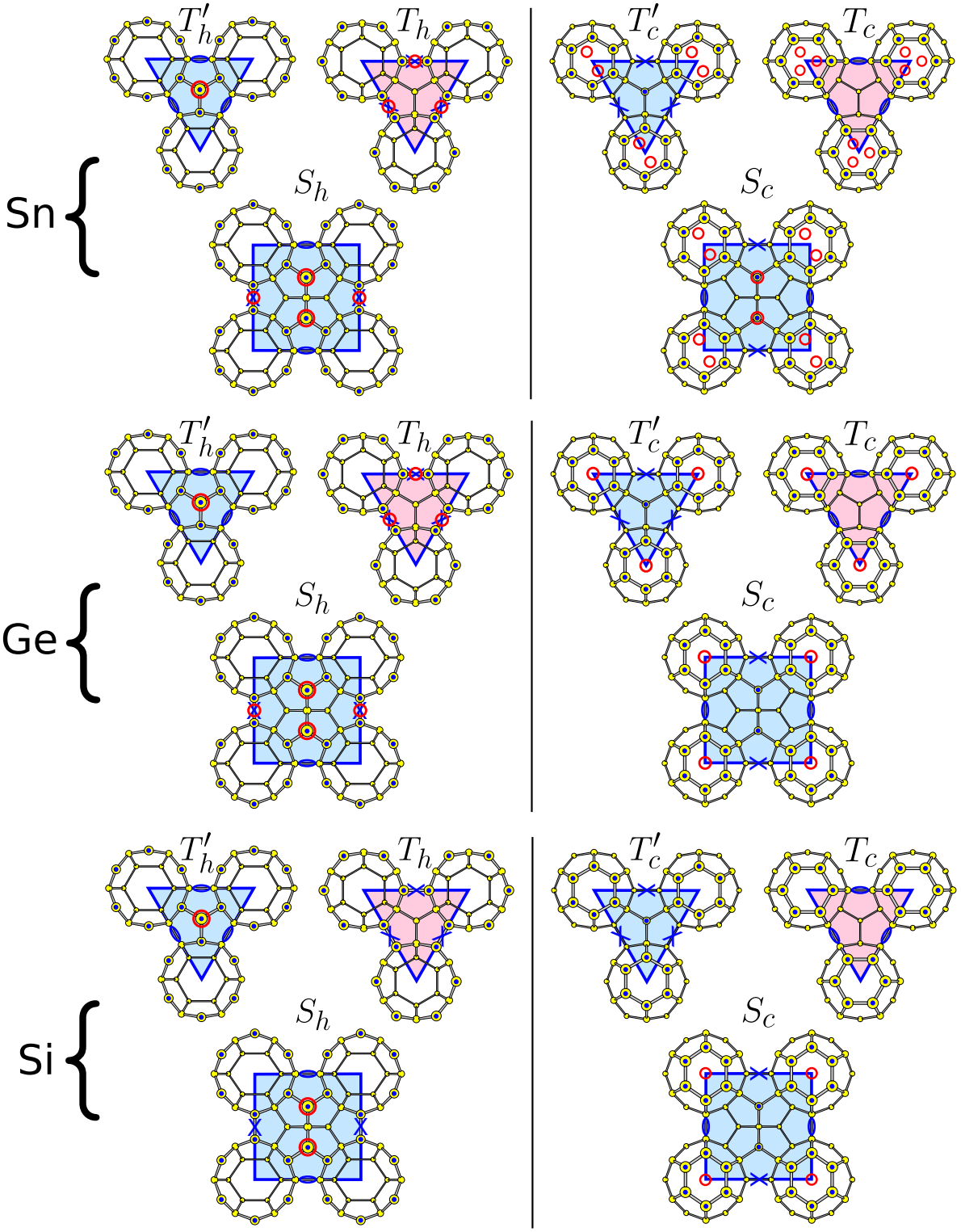

Figure S3.1: Optimal reconstruction of *dodecagonal* Sn, Ge and Si clathrate tiles: equilateral triangle (T) and square (S) terminated by cage "caps" (c) and "holes" (h). For the explanation of the symbols and color scheme, consult Figure S2.1. Note that placing the "caps" on the top of the "holes" does not change the number of unsaturated 3-coordinated atoms (distinguished by blue central dots); this holds also for the decagonal cases, see Figure S2.1.

S4. Reconstructed vs. Unreconstructed Surfaces

Figures S4.1 and S4.3 below implies that Sn and Si clathrate slabs possess clear energetic advantage over the corresponding (111)-diamond films of the same coverage already *before* surface reconstruction (addition of Si atoms to the slab's surface followed by atomic-position DFT relaxation). However, the appropriate surface reconstruction is responsible for further energy decrease of clathrates with respect to the diamond rivals.

Notably, as can be observed in Figure S4.2, the opposite situation happens for Ge, where clathrate's internal-energy advantage over diamond is markedly more pronounced for the *unreconstructed* slabs.

In all the graphs below, the region of clathrate film stability is highlighted by green shadow, compare with Figure 6 of the main text. Reconstructed slabs correspond to the unreconstructed structures ("reconstructed" = "unreconstructed" + adatoms) in each case. As for the reconstructed ones, the most stable clathrate and diamond films for each coverage ρ from Figure 6 of the main text were chosen for comparison, confer Results section.

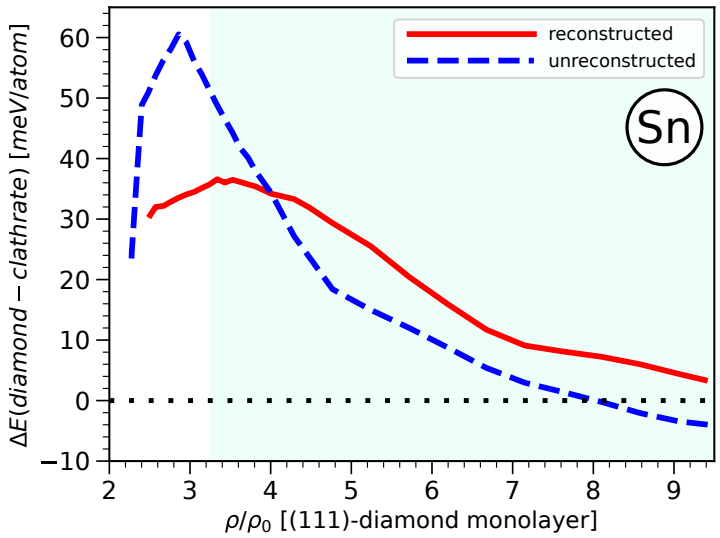

Figure S4.1: Comparison of per-atom energy difference between the most stable Sn clathrate slabs and Sn (111)-diamond ones for reconstructed and unreconstructed case.

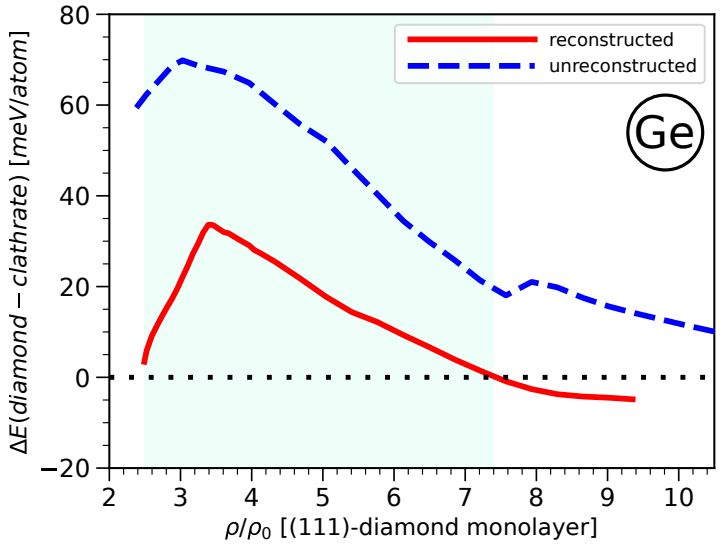

Figure S4.2: Comparison of per-atom energy difference between the most stable Ge clathrate slabs and Ge (111)-diamond ones for reconstructed and unreconstructed case.

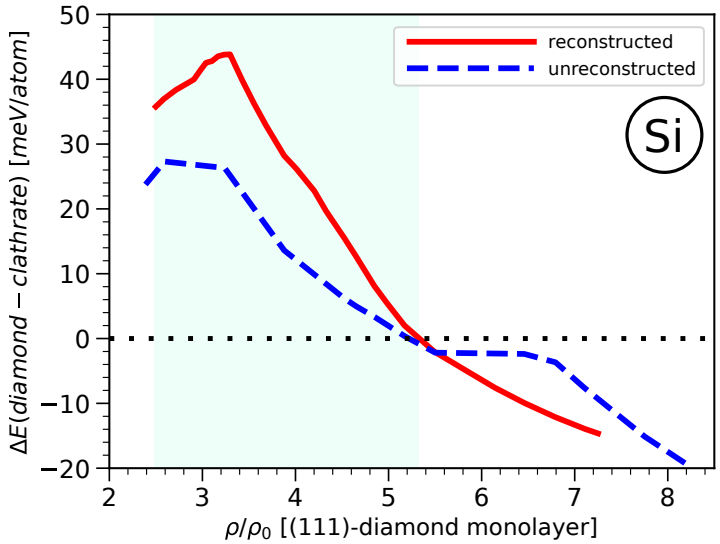

Figure S4.3: Comparison of per-atom energy difference between the most stable Si clathrate slabs and Si (111)-diamond ones for reconstructed and unreconstructed case.

S5. Comparison of Various Types of Clathrate Slabs

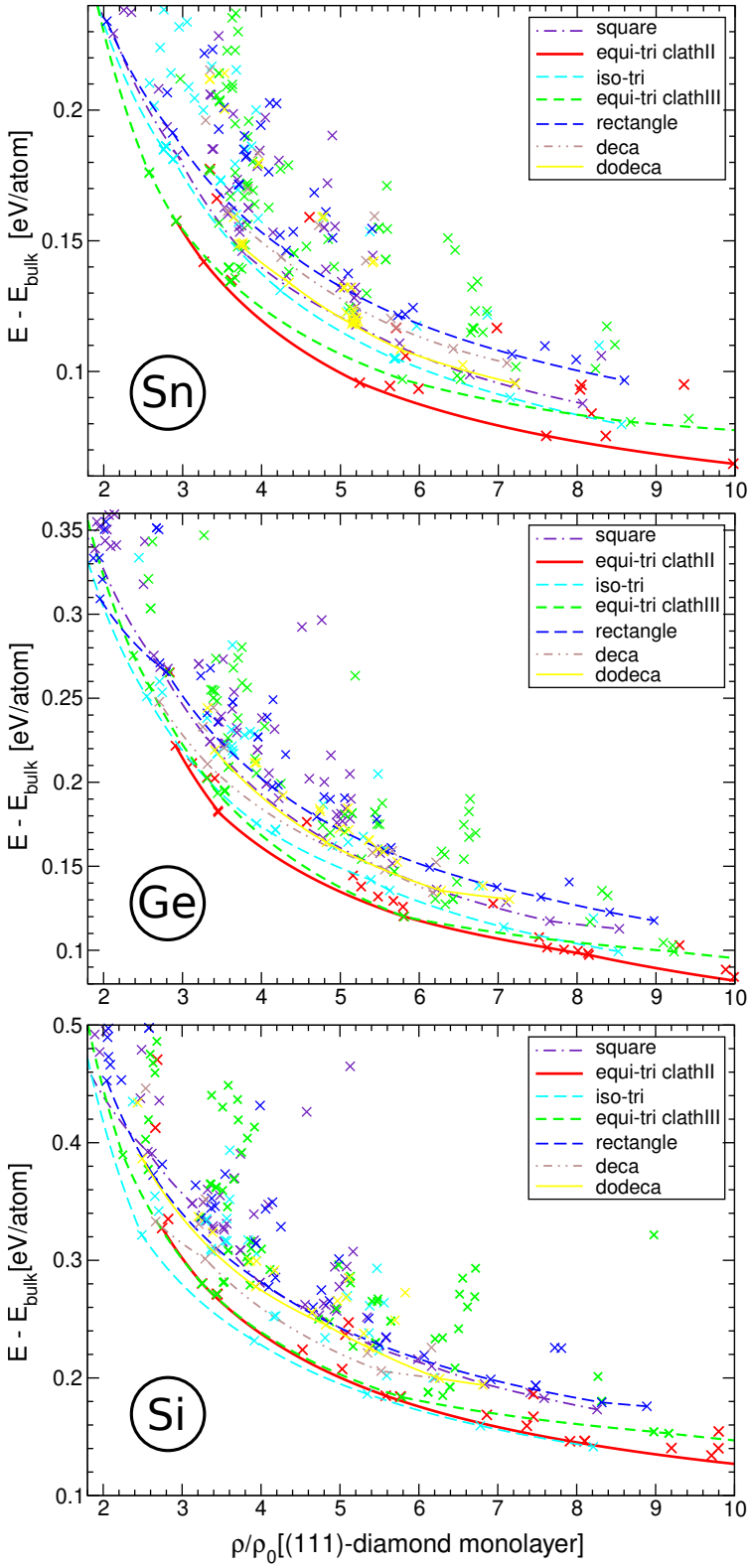

Figure S5.1: Stability comparison (DFT energy per atom at 0K) of seven types of Sn, Ge and Si clathrate thin films: clath-I square, clath-II equilateral triangle, clath-II isosceles triangle, clath-III equilateral triangle and rectangle, decagonal and clath-IV dodecagonal tiling reconstructed according to Figures S2.1, S3.1. Each cross represents one attempt for clath-tile reconstruction.

S6. Crystallization of Clathrate Slabs from the Melt

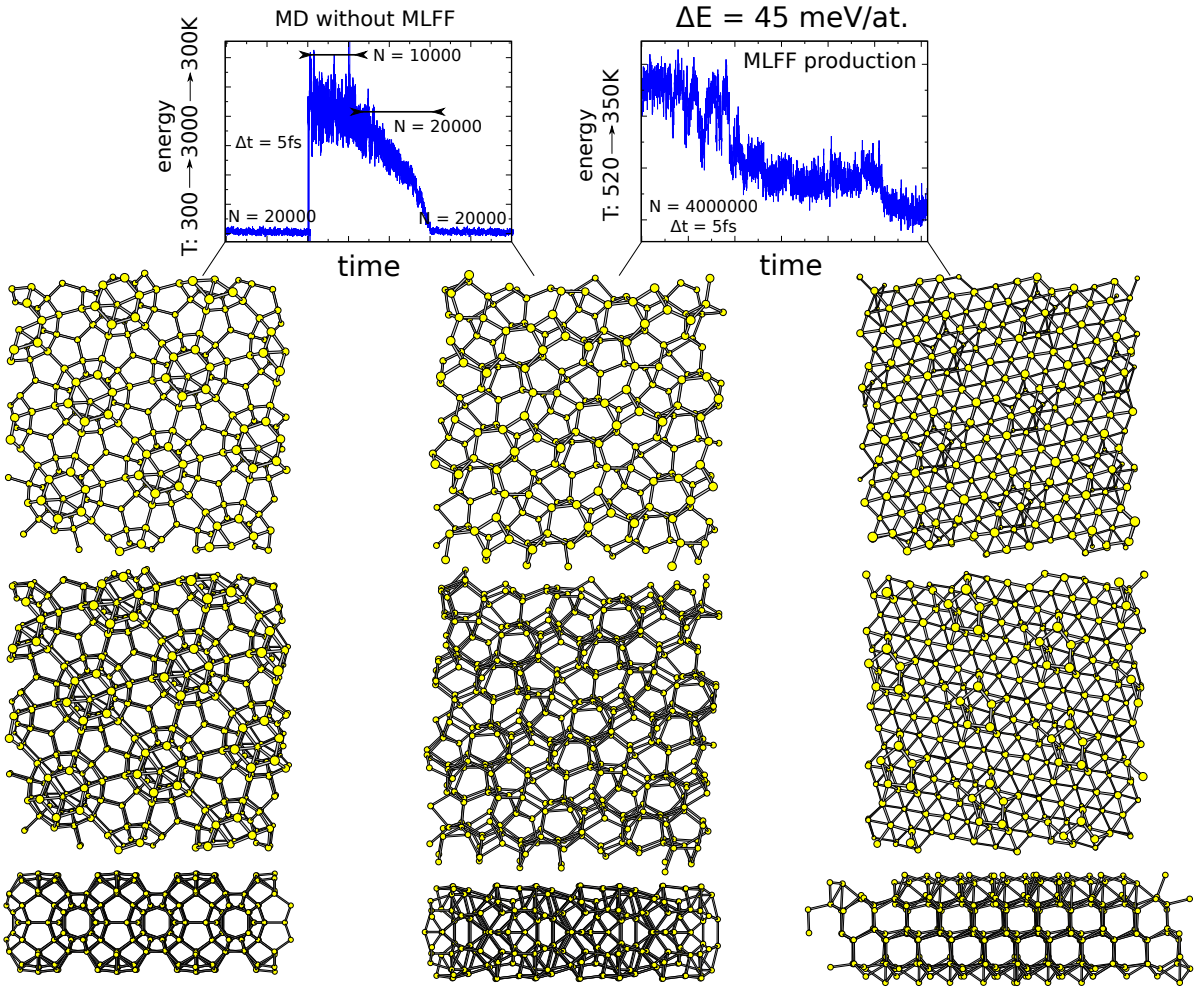

Figure S6.1: Spontaneous re-crystallization of free-standing initially symmetrical Ge film, sample designated as Ge.equi-II-3.5 in the main text, see Subsubsection S9.2.4 for the atomic coordinates.

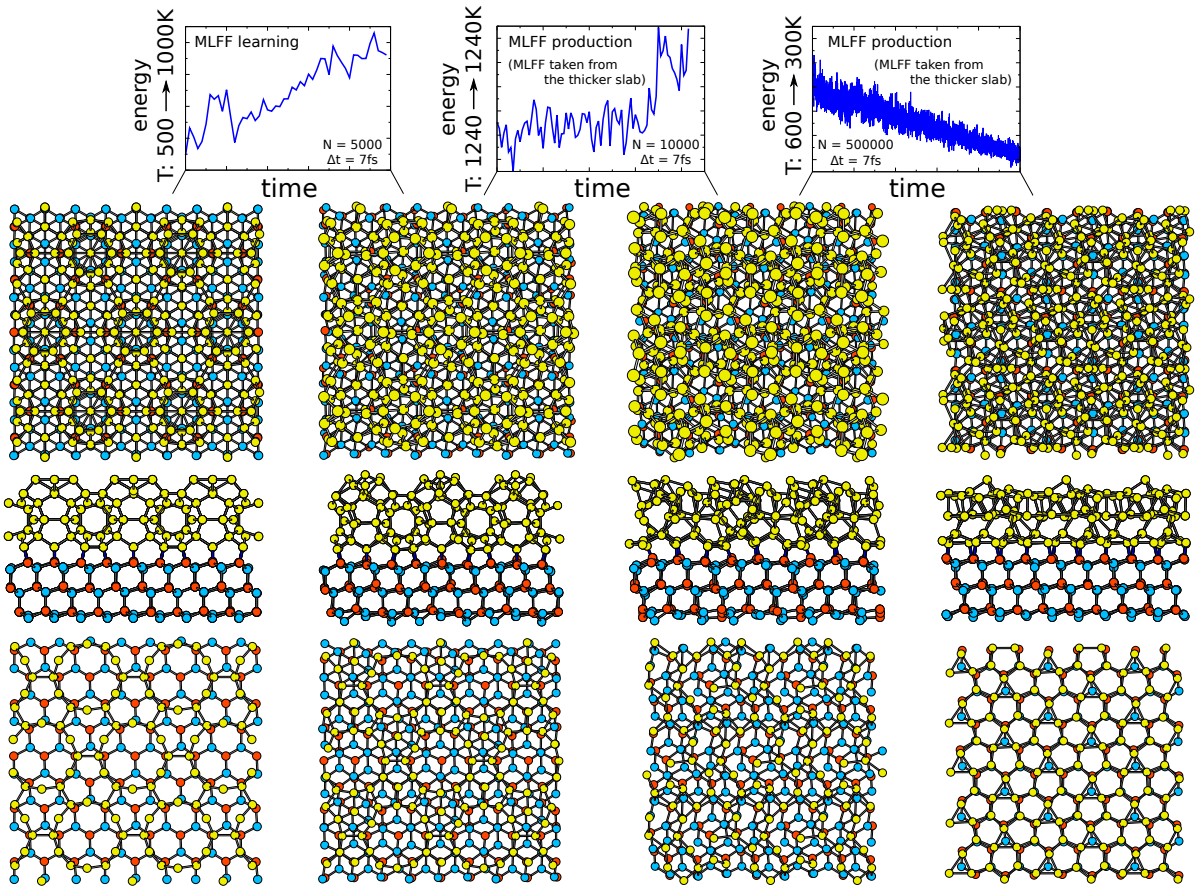

Figure S6.2: Spontaneous re-crystallization of Ge films on InN. Starting from the thinnest clathrate film with 6-caps, see Subsubsection S9.4.1 for the atomic coordinates.

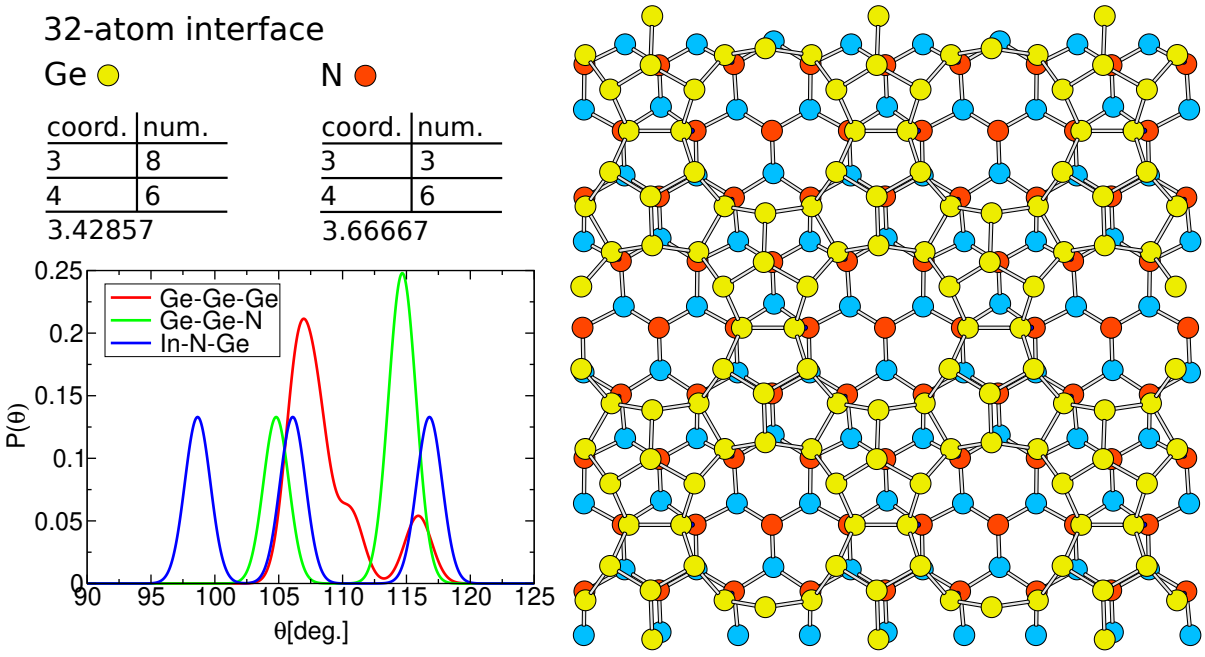

Figure S6.3: Coherent clathrate/diamond interface made up of Ge/InN.

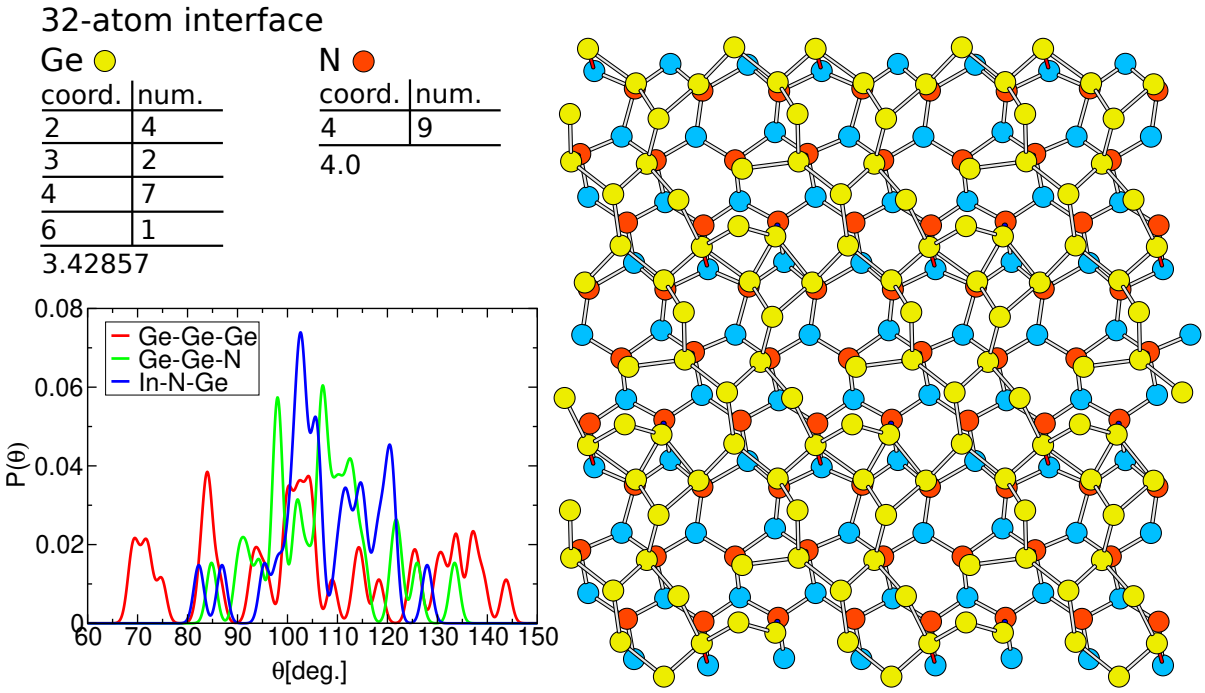

Figure S6.4: Interface between diamond and clathrate melt after $N = 10000$ d$t = 7$ fs-steps at 1240 K, according to roadmap S6.2.

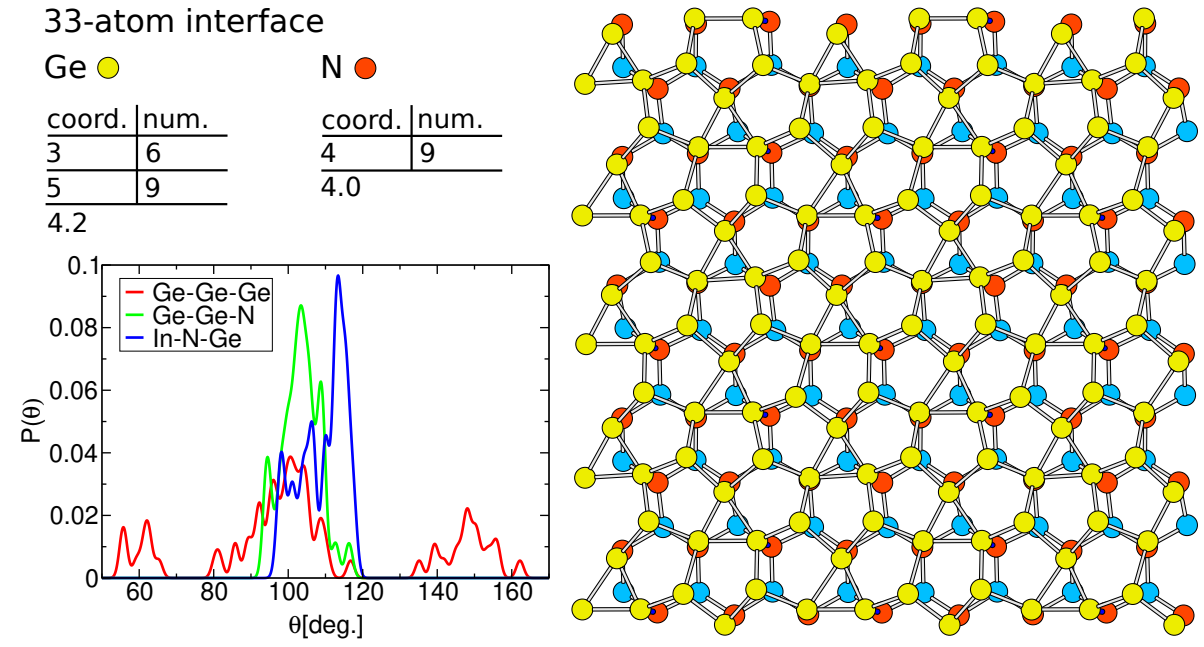

Figure S6.5: Interface between diamond and re-crystallized clathrate melt according to Figure S6.2.

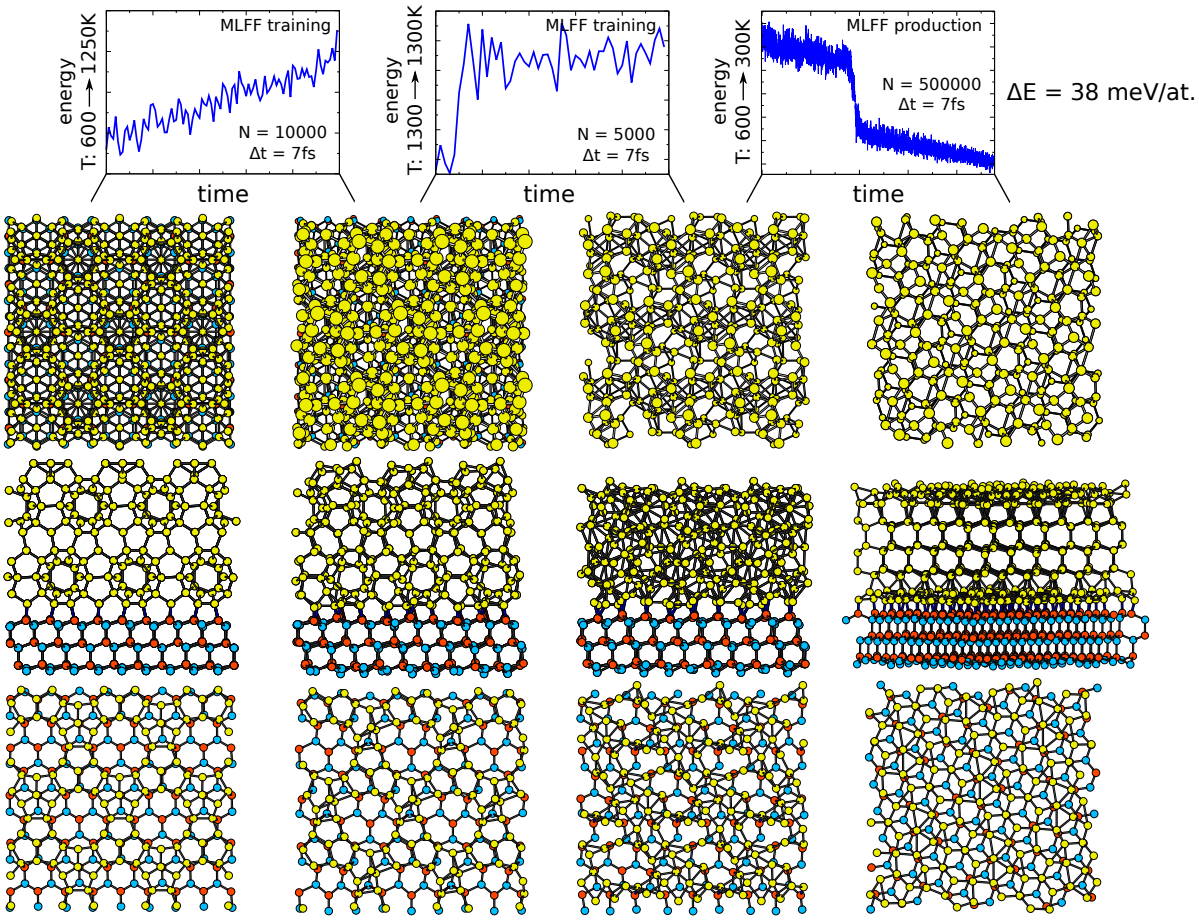

Figure S6.6: Spontaneous re-crystallization of Ge films on InN. Starting from thicker clathrate film with 6-caps, see Subsubsection S9.4.2 for the atomic coordinates.

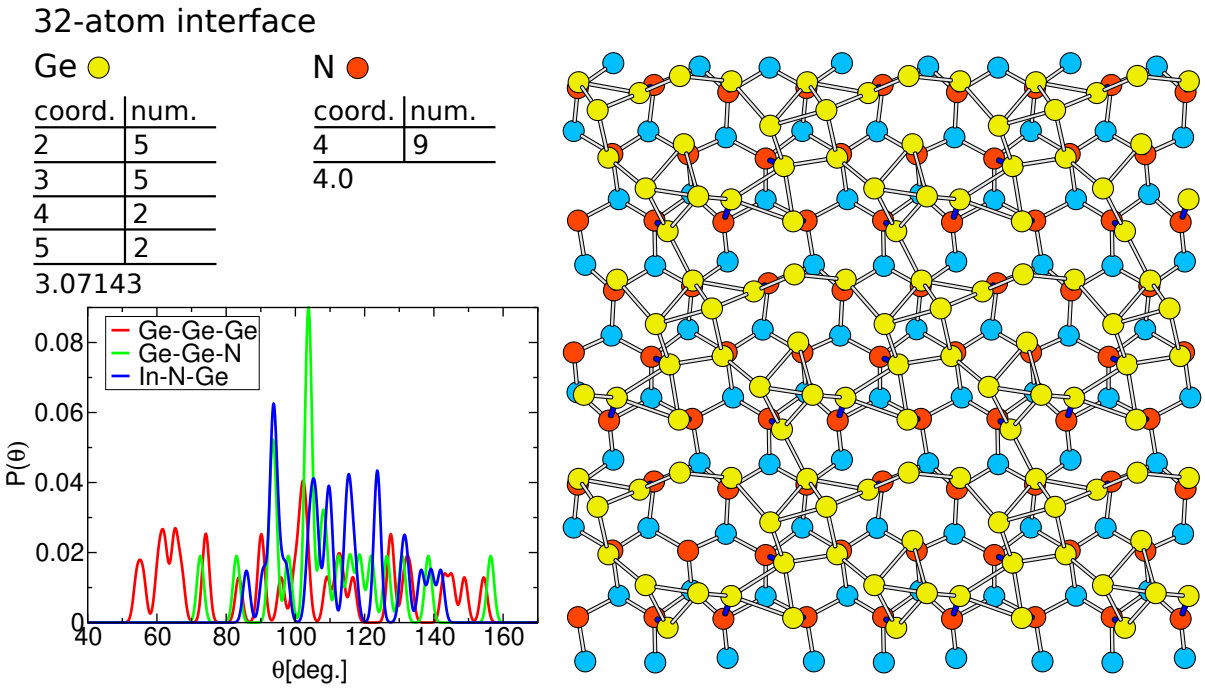

Figure S6.7: Interface between diamond and clathrate melt after $N = 5000$ d$t = 7$ fs-steps at 1300 K, according to Figure S6.6.

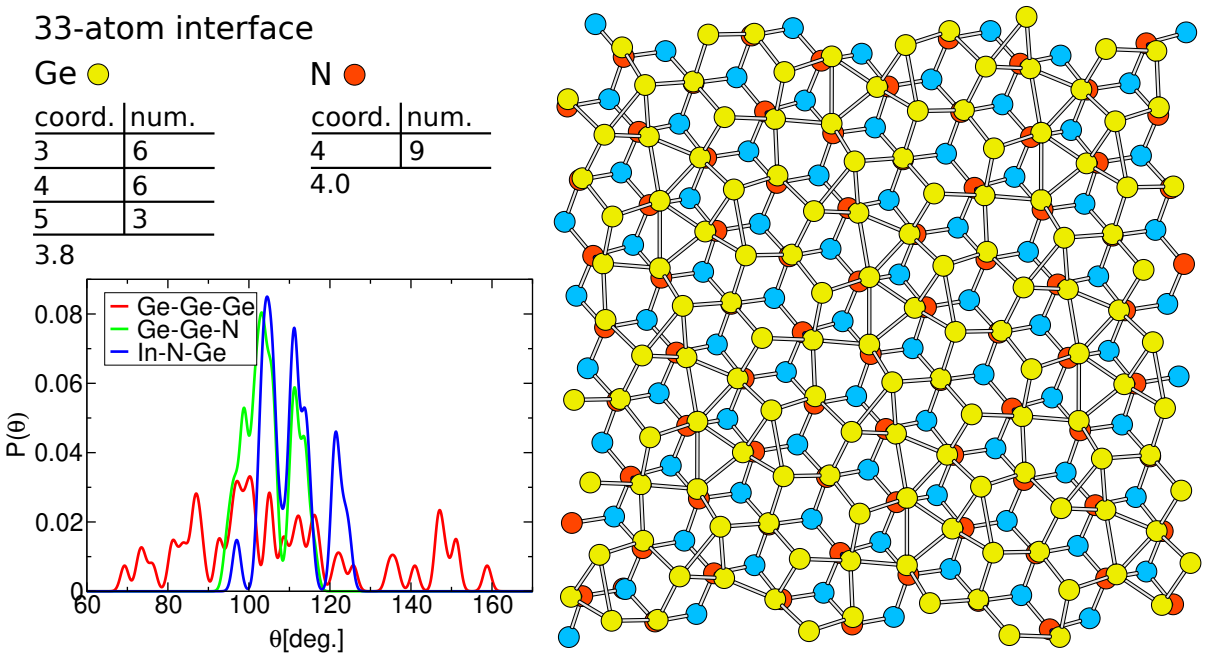

Figure S6.8: Interface between diamond and re-crystallized clathrate melt according to Figure S6.6.

S7. van der Waals Dispersion Correction of G4 Slabs

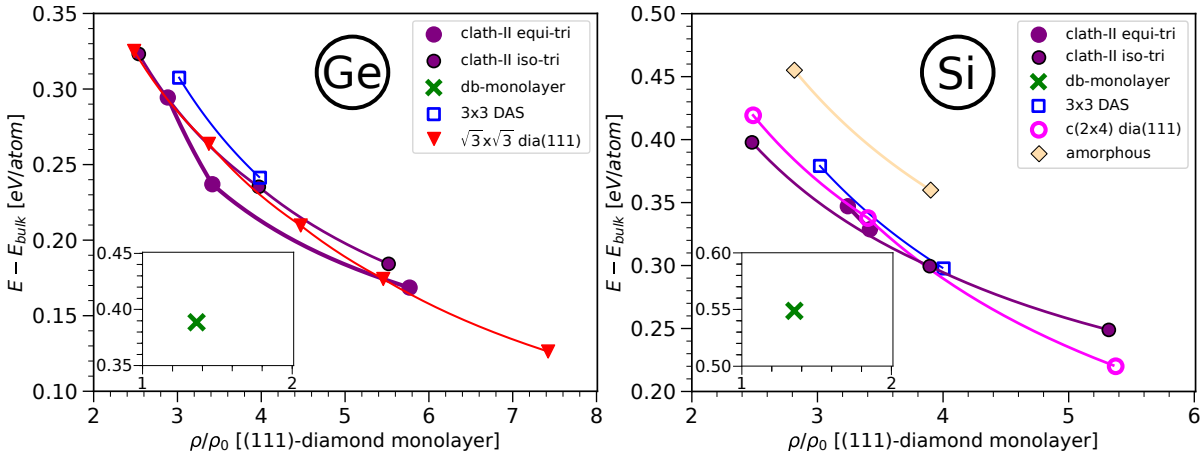

Figure S7.1: Change of the diamond-clathrate stability competition in response to the van der Waals dispersion correction PBE-D3 (`ivdw=12`), visit Subsection 6.4 in the main text.

S8. Electronic Density of States: Clathrate Slabs & Bulk

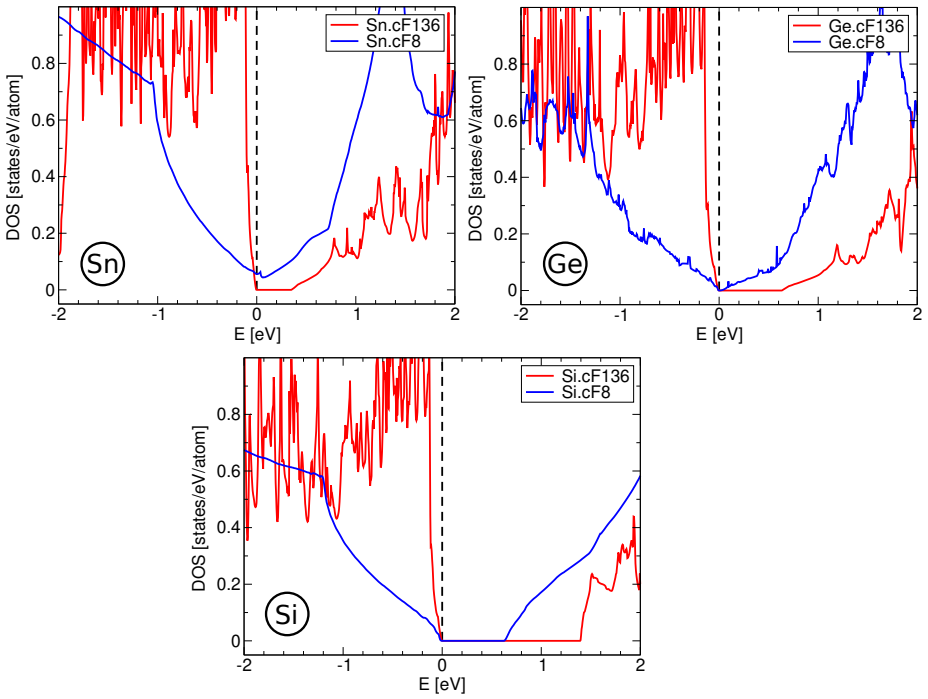

Figure S8.1: Electronic Density of States, eDOS, of the bulk type-II clathrates (cF136) compared with bulk diamond (cF8) for Sn, Ge and Si. Fermi energy, E_F, is designated by the vertical thick dashed line.

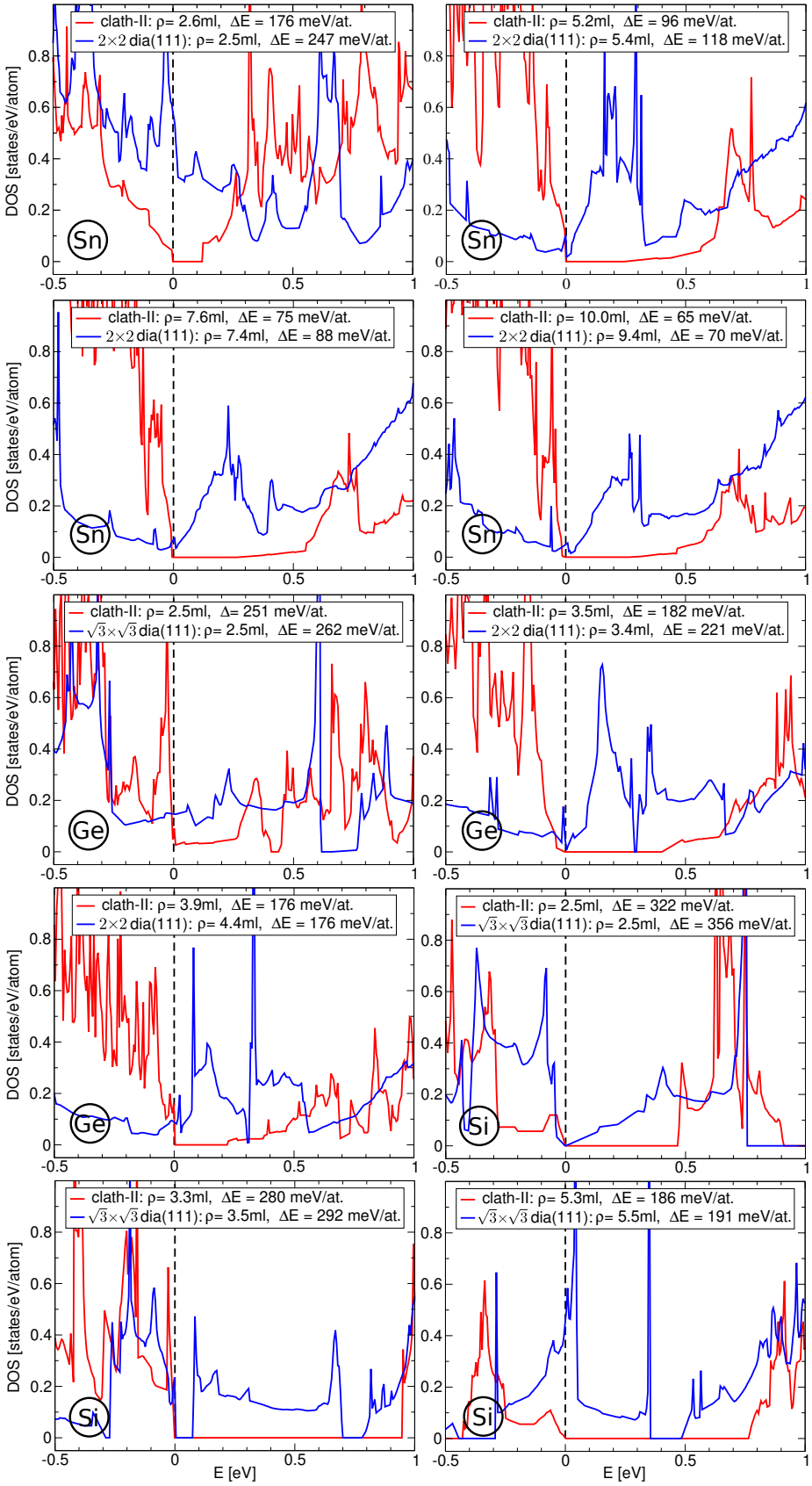

Figure S8.2: Electronic Density of States, eDOS, of the most stable clathrate slabs, compared with that of the competitive diamond slabs of approximately the same thickness ρ. Fermi energy, E_F, is designated by vertical thick dashed line. Visit Subsection 5.4 in the main text.

S9. xyz Files

S9.1 Tin-Slab xyz Files

S9.1.1 Sn9-web

$\rho = 0.1749\,\text{Å}^{-2} = 1.667\,\text{ML}$, $E - E_{\text{bulk}} = 216\,\text{meV/at.}$

```
23.9138     0.00000   0.00000
0.00000     23.9138   0.00000
0.00000     0.00000   23.9138
100 atoms
0.96713     0.89507   0.02979   50   1    1
0.18163     0.30665   0.95156   50   2    2
0.00243     0.36734   0.04387   50   3    3
0.11868     0.91534   0.92111   50   4    4
0.18669     0.44073   0.96766   50   5    5
0.12692     0.38930   0.86865   50   6    6
0.81752     0.94640   0.91512   50   7    7
0.22004     0.78823   0.05703   50   8    8
0.88308     0.80335   0.06302   50   9    9
0.94704     0.92053   0.90656   50   10   10
0.08813     0.54847   0.12274   50   11   11
0.30671     0.70521   0.98685   50   12   12
0.04241     0.44174   0.94857   50   13   13
0.19810     0.35715   0.06952   50   14   14
0.86364     0.84115   0.85282   50   15   15
0.19066     0.17224   0.99467   50   16   16
0.42224     0.74919   0.03300   50   17   17
0.70438     0.93414   0.08492   50   18   18
0.54387     0.91304   0.98796   50   19   19
0.90148     0.00005   0.99533   50   20   20
0.44552     0.17554   0.93494   50   21   21
0.89188     0.65382   0.08673   50   22   22
0.08124     0.15403   0.07424   50   23   23
0.64025     0.85720   0.16452   50   24   24
0.93849     0.79543   0.94609   50   25   25
0.68329     0.64525   0.96937   50   26   26
0.98708     0.10118   0.00128   50   27   27
0.88829     0.53527   0.14043   50   28   28
0.07818     0.01873   0.03478   50   29   29
0.42503     0.29041   0.08684   50   30   30
0.24033     0.95059   0.90392   50   31   31
0.62870     0.00321   0.00457   50   32   32
0.18179     0.07626   0.08287   50   33   33
0.36438     0.36431   0.89509   50   34   34
0.98208     0.56142   0.06184   50   35   35
```

0.69423	0.89719	0.96087	50	36	36
0.50253	0.38736	0.05731	50	37	37
0.45773	0.04332	0.91417	50	38	38
0.82545	0.91695	0.04931	50	39	39
0.55073	0.81738	0.08054	50	40	40
0.06642	0.18467	0.94560	50	41	41
0.34977	0.85690	0.04637	50	42	42
0.10212	0.43689	0.07187	50	43	43
0.16142	0.63510	0.06777	50	44	44
0.80136	0.82302	0.96140	50	45	45
0.61960	0.67539	0.07927	50	46	46
0.10048	0.74935	0.06073	50	47	47
0.35541	0.10422	0.87435	50	48	48
0.77326	0.70727	0.90756	50	49	49
0.35139	0.54493	0.98922	50	50	50
0.44485	0.62899	0.97813	50	51	51
0.68230	0.80690	0.05652	50	52	52
0.60103	0.80739	0.95993	50	53	53
0.83374	0.50991	0.93448	50	54	54
0.09770	0.28042	0.05107	50	55	55
0.25804	0.82722	0.93791	50	56	56
0.23032	0.91394	0.03167	50	57	57
0.97614	0.66315	0.98586	50	58	58
0.45375	0.91336	0.09431	50	59	59
0.85835	0.63266	0.95822	50	60	60
0.32438	0.36599	0.10798	50	61	61
0.38238	0.80974	0.92592	50	62	62
0.31187	0.42331	0.99262	50	63	63
0.04016	0.95712	0.83578	50	64	64
0.42334	0.92829	0.96173	50	65	65
0.06181	0.05552	0.90817	50	66	66
0.77760	0.71842	0.03918	50	67	67
0.10963	0.54441	0.98974	50	68	68
0.23181	0.60240	0.95877	50	69	69
0.68340	0.56369	0.06703	50	70	70
0.17041	0.71722	0.95411	50	71	71
0.52931	0.10250	0.00184	50	72	72
0.28299	0.61421	0.08203	50	73	73
0.18144	0.04656	0.96071	50	74	74
0.09489	0.89037	0.04486	50	75	75
0.16146	0.80502	0.86034	50	76	76
0.90454	0.46266	0.03091	50	77	77
0.57583	0.95224	0.11153	50	78	78
0.44658	0.44157	0.95606	50	79	79
0.56200	0.68418	0.96535	50	80	80
0.95951	0.54163	0.93519	50	81	81
0.33026	0.08375	0.08606	50	82	82
0.44012	0.03100	0.05198	50	83	83
0.80761	0.55570	0.04933	50	84	84
0.32017	0.73529	0.11244	50	85	85

0.33400	0.29204	0.99652	50	86	86
0.67111	0.52100	0.93956	50	87	87
0.41257	0.58602	0.10125	50	88	88
0.06569	0.80185	0.94906	50	89	89
0.04873	0.31091	0.93358	50	90	90
0.33098	0.02608	0.97160	50	91	91
0.40518	0.46092	0.08388	50	92	92
0.45882	0.30776	0.96075	50	93	93
0.43056	0.16401	0.06316	50	94	94
0.61008	0.61374	0.87023	50	95	95
0.32467	0.16033	0.98493	50	96	96
0.53509	0.53990	0.93945	50	97	97
0.53490	0.58237	0.06596	50	98	98
0.15668	0.13509	0.87445	50	99	99
0.59489	0.47624	0.03422	50	100	100

S9.1.2 triangles
$\rho = 0.2225$ Å$^{-2} = 2.121$ ML, $E - E_{\text{bulk}} = 198$ meV/at.

3.55789	-0.00806	0.00000			
-3.56552	4.68674	0.00000			
0.00000	0.00000	28.0000			
4 atoms					
0	0.25	0.07803	50	1	1
0	0.75	0.92197	50	2	2
0	0.25	0.96739	50	3	3
0	0.75	0.03261	50	4	4

S9.1.3 squares
$\rho = 0.2448$ Å$^{-2} = 2.333$ ML, $E - E_{\text{bulk}} = 158$ meV/at.

5.72637	0.00000	0.00000			
0.00000	5.72637	0.00000			
0.00000	0.00000	20.5771			
8 atoms					
0	0	0.56989	50	1	1
0.5	0.5	0.56989	50	2	2
0	0	0.41700	50	3	3
0.5	0.5	0.41700	50	4	4
0	0.5	0.62798	50	5	5
0.5	0	0.35890	50	6	6
0	0.5	0.47756	50	7	7
0.5	0	0.50932	50	8	8

S9.1.4 Sn.equi-II-3
$\rho = 0.3428$ Å$^{-2} = 3.268$ ML, $E - E_{\text{bulk}} = 142$ meV/at.

12.44832 -0.00000 -0.00008
-6.22416 10.78059 -0.00011
-0.00022 -0.00049 34.25425
46 atoms
0.33338 0.05896 0.26941 50 1 1
0.94107 0.27436 0.26942 50 2 2
0.72567 0.66667 0.26941 50 3 3
0.70092 0.03421 0.26532 50 4 4
0.33337 0.29911 0.26533 50 5 5
0.96582 0.66667 0.26533 50 6 6
0.95506 0.28834 0.02648 50 7 7
0.33331 0.04491 0.02648 50 8 8
0.71162 0.66659 0.02648 50 9 9
0.33332 0.28934 0.02653 50 10 10
0.71067 0.04395 0.02652 50 11 11
0.95605 0.66661 0.02653 50 12 12
0.53980 0.46057 0.07974 50 13 13
0.53938 0.07916 0.07972 50 14 14
0.92083 0.46015 0.07974 50 15 15
0.75269 0.87046 0.21963 50 16 16
0.11783 0.24731 0.21964 50 17 17
0.12956 0.88219 0.21964 50 18 18
1.00000 0.99995 0.10916 50 19 19
0.66670 0.33332 0.19192 50 20 20
0.54890 0.46285 0.21964 50 21 21
0.53716 0.08599 0.21963 50 22 22
0.91402 0.45112 0.21965 50 23 23
0.74587 0.87267 0.07972 50 24 24
0.12686 0.25411 0.07975 50 25 25
0.12729 0.87309 0.07974 50 26 26
0.00003 0.99999 0.19192 50 27 27
0.66667 0.33329 0.10916 50 28 28
0.46594 0.53418 0.15057 50 29 29
0.46583 0.93171 0.15056 50 30 30
0.06830 0.53407 0.15058 50 31 31
0.59842 0.79912 0.15056 50 32 32
0.20077 0.40159 0.15058 50 33 33
0.20089 0.79923 0.15057 50 34 34
0.07730 0.41060 0.34526 50 35 35
0.12885 0.66668 0.32593 50 36 36
0.33338 0.46215 0.32593 50 37 37
0.33339 0.92276 0.34525 50 38 38
0.58947 0.66668 0.34525 50 39 39
0.53791 0.87120 0.32592 50 40 40
0.19051 0.52380 0.26067 50 41 41
0.33337 0.80952 0.26066 50 42 42
0.47623 0.66666 0.26066 50 43 43
0.83399 0.66656 0.10590 50 44 44
0.83265 0.16593 0.10590 50 45 45
0.33327 0.16728 0.10590 50 46 46

S9.1.5 Sn.equi-II-5
$\rho = 0.5501$ Å$^{-2} = 5.244$ ML, $E - E_{\mathrm{bulk}} = 96$ meV/at.

12.46276	0.00004	0.00003			
-6.23135	10.79309	-0.00004			
0.00009	-0.00009	41.74180			
74 atoms					
0.33759	0.05312	0.21120	50	1	1
0.94690	0.28451	0.21120	50	2	2
0.71549	0.66242	0.21120	50	3	3
0.71549	0.05310	0.21120	50	4	4
0.33758	0.28451	0.21120	50	5	5
0.94688	0.66241	0.21120	50	6	6
0.95688	0.28649	0.01775	50	7	7
0.32957	0.04308	0.01775	50	8	8
0.71350	0.67043	0.01775	50	9	9
0.32957	0.28649	0.01775	50	10	10
0.71350	0.04311	0.01775	50	11	11
0.95692	0.67043	0.01775	50	12	12
0.61782	0.61360	0.27509	50	13	13
0.99573	0.38219	0.27509	50	14	14
0.38642	0.00428	0.27509	50	15	15
0.99572	0.61358	0.27509	50	16	16
0.38640	0.38218	0.27509	50	17	17
0.61781	0.00427	0.27509	50	18	18
0.53981	0.46019	0.06000	50	19	19
0.53981	0.07966	0.06000	50	20	20
0.92034	0.46019	0.06000	50	21	21
0.20780	0.79221	0.30980	50	22	22
0.20780	0.41564	0.30981	50	23	23
0.58436	0.79220	0.30981	50	24	24
0.74895	0.87449	0.17649	50	25	25
0.12551	0.25105	0.17649	50	26	26
0.12551	0.87449	0.17649	50	27	27
0.99999	0.00001	0.08775	50	28	28
0.66665	0.33335	0.33446	50	29	29
0.66665	0.33334	0.15183	50	30	30
0.54290	0.45710	0.17347	50	31	31
0.54290	0.08584	0.17347	50	32	32
0.91416	0.45710	0.17347	50	33	33
0.74857	0.87430	0.06230	50	34	34
0.12570	0.25143	0.06230	50	35	35
0.12570	0.87430	0.06230	50	36	36
0.41914	0.20960	0.31282	50	37	37
0.79040	0.58086	0.31282	50	38	38
0.79041	0.20960	0.31282	50	39	39
0.99999	0.00001	0.15577	50	40	40

0.66665	0.33335	0.08417	50	41	41
0.33332	0.66668	0.33051	50	42	42
0.46549	0.53451	0.11781	50	43	43
0.46549	0.93101	0.11781	50	44	44
0.06899	0.53451	0.11781	50	45	45
0.13203	0.86797	0.36675	50	46	46
0.13204	0.26412	0.36675	50	47	47
0.73588	0.86797	0.36675	50	48	48
0.59743	0.79873	0.11954	50	49	49
0.20127	0.40256	0.11954	50	50	50
0.20127	0.79873	0.11955	50	51	51
0.00375	0.38021	0.46855	50	52	52
0.61980	0.62359	0.46855	50	53	53
0.37638	0.99625	0.46855	50	54	54
0.37641	0.38021	0.46855	50	55	55
0.00375	0.62362	0.46855	50	56	56
0.61980	0.99625	0.46855	50	57	57
0.41297	0.20651	0.42629	50	58	58
0.79349	0.58703	0.42629	50	59	59
0.79349	0.20651	0.42630	50	60	60
0.33332	0.66668	0.39854	50	61	61
0.20761	0.79239	0.42399	50	62	62
0.20762	0.41528	0.42399	50	63	63
0.58472	0.79238	0.42399	50	64	64
0.66666	0.33335	0.40212	50	65	65
0.26433	0.13219	0.36849	50	66	66
0.86781	0.73567	0.36849	50	67	67
0.86781	0.13219	0.36849	50	68	68
0.33339	0.16671	0.08294	50	69	69
0.83328	0.16672	0.08294	50	70	70
0.83329	0.66661	0.08294	50	71	71
0.50003	0.49997	0.40335	50	72	72
0.99991	0.49998	0.40336	50	73	73
0.50002	0.00010	0.40336	50	74	74

S9.1.6 Sn.equi-II-7.5

$\rho = 0.7981$ Å$^{-2} = 7.608$ ML, $E - E_{\text{bulk}} = 75$ meV/at.

12.50059	-0.00001	0.00007			
-6.25030	10.82582	-0.00009			
0.00033	-0.00026	52.72611			
108 atoms					
0.33844	0.05386	0.16954	50	1	1
0.94615	0.28458	0.16954	50	2	2
0.71543	0.66156	0.16954	50	3	3
0.29003	0.95257	0.82048	50	4	4
0.66258	0.70993	0.82048	50	5	5

0.04743	0.33741	0.82048	50	6	6
0.66258	0.95257	0.82048	50	7	7
0.04742	0.70996	0.82048	50	8	8
0.29006	0.33742	0.82048	50	9	9
0.71542	0.05385	0.16954	50	10	10
0.33844	0.28458	0.16954	50	11	11
0.94614	0.66156	0.16954	50	12	12
0.95126	0.27947	0.02386	50	13	13
0.32823	0.04874	0.02386	50	14	14
0.72054	0.67177	0.02386	50	15	15
0.32823	0.27945	0.02386	50	16	16
0.72053	0.04874	0.02386	50	17	17
0.95125	0.67177	0.02386	50	18	18
0.67146	0.72021	0.97325	50	19	19
0.27980	0.95121	0.97325	50	20	20
0.04879	0.32854	0.97325	50	21	21
0.61790	0.61313	0.22015	50	22	22
0.99522	0.38211	0.22015	50	23	23
0.38689	0.00478	0.22015	50	24	24
0.99522	0.61311	0.22015	50	25	25
0.38688	0.38210	0.22015	50	26	26
0.61789	0.00478	0.22015	50	27	27
0.04878	0.72020	0.97325	50	28	28
0.67145	0.95120	0.97325	50	29	29
0.27978	0.32854	0.97325	50	30	30
0.54130	0.45870	0.05090	50	31	31
0.54130	0.08258	0.05090	50	32	32
0.91742	0.45870	0.05090	50	33	33
0.08230	0.54113	0.94596	50	34	34
0.45887	0.91770	0.94596	50	35	35
0.45887	0.54113	0.94596	50	36	36
0.20781	0.79220	0.24744	50	37	37
0.20780	0.41562	0.24744	50	38	38
0.58439	0.79220	0.24744	50	39	39
0.74926	0.87463	0.14250	50	40	40
0.12538	0.25074	0.14250	50	41	41
0.12538	0.87462	0.14250	50	42	42
0.87338	0.12662	0.85368	50	43	43
0.87338	0.74671	0.85368	50	44	44
0.25328	0.12662	0.85368	50	45	45
0.00001	0.99999	0.07199	50	46	46
0.00001	0.99998	0.92623	50	47	47
0.66666	0.33334	0.26717	50	48	48
0.66667	0.33333	0.12142	50	49	49
0.33335	0.66665	0.87583	50	50	50
0.54361	0.45639	0.13955	50	51	51
0.54361	0.08720	0.13955	50	52	52
0.91280	0.45640	0.13955	50	53	53
0.08246	0.54121	0.85570	50	54	54
0.45879	0.91754	0.85570	50	55	55

0.45879	0.54120	0.85571	50	56	56
0.75388	0.87693	0.05385	50	57	57
0.12307	0.24612	0.05385	50	58	58
0.12307	0.87693	0.05385	50	59	59
0.87645	0.12355	0.94334	50	60	60
0.87645	0.75286	0.94334	50	61	61
0.24714	0.12355	0.94334	50	62	62
0.41952	0.20977	0.25007	50	63	63
0.79024	0.58048	0.25007	50	64	64
0.79024	0.20977	0.25007	50	65	65
0.00001	1.00000	0.12575	50	66	66
0.00001	0.99999	0.87267	50	67	67
0.66667	0.33333	0.06766	50	68	68
0.33335	0.66665	0.92969	50	69	69
0.33333	0.66667	0.26371	50	70	70
0.46514	0.53486	0.09582	50	71	71
0.46514	0.93025	0.09582	50	72	72
0.06975	0.53487	0.09582	50	73	73
0.93045	0.46520	0.90088	50	74	74
0.53480	0.06955	0.90088	50	75	75
0.53480	0.46520	0.90088	50	76	76
0.13187	0.86813	0.29252	50	77	77
0.13187	0.26376	0.29252	50	78	78
0.73625	0.86813	0.29252	50	79	79
0.59693	0.79846	0.09758	50	80	80
0.20154	0.40307	0.09758	50	81	81
0.20154	0.79846	0.09758	50	82	82
0.79876	0.20123	0.89937	50	83	83
0.79876	0.59748	0.89937	50	84	84
0.40252	0.20123	0.89937	50	85	85
0.00414	0.38078	0.37293	50	86	86
0.61923	0.62337	0.37292	50	87	87
0.37660	0.99587	0.37292	50	88	88
0.37663	0.38077	0.37292	50	89	89
0.00414	0.62340	0.37293	50	90	90
0.61923	0.99587	0.37293	50	91	91
0.41341	0.20671	0.33973	50	92	92
0.79330	0.58660	0.33973	50	93	93
0.79329	0.20671	0.33973	50	94	94
0.33333	0.66667	0.31756	50	95	95
0.20789	0.79212	0.33769	50	96	96
0.20789	0.41579	0.33769	50	97	97
0.58421	0.79212	0.33769	50	98	98
0.66667	0.33334	0.32073	50	99	99
0.26417	0.13209	0.29404	50	100	100
0.86791	0.73584	0.29404	50	101	101
0.86791	0.13209	0.29405	50	102	102
0.16674	0.33343	0.87209	50	103	103
0.66656	0.83325	0.87209	50	104	104
0.16673	0.83327	0.87209	50	105	105

0.49994	0.50006	0.32131	50	106	106
0.00013	0.50007	0.32132	50	107	107
0.49993	0.99988	0.32132	50	108	108

S9.1.7 Sn.equi-II-10

$\rho = 1.047$ Å$^{-2} = 9.978$ ML, $E - E_{\mathrm{bulk}} = 65$ meV/at.

12.51618	0.00000	0.00000			
-6.25809	10.83933	0.00000			
0.00000	0.00000	62.18220			
142 atoms					
0.33865	0.05400	0.14502	50	1	1
0.94600	0.28466	0.14502	50	2	2
0.71534	0.66135	0.14502	50	3	3
0.28466	0.94600	0.85498	50	4	4
0.66135	0.71534	0.85498	50	5	5
0.05400	0.33865	0.85498	50	6	6
0.66135	0.94600	0.85498	50	7	7
0.05400	0.71534	0.85498	50	8	8
0.28466	0.33865	0.85498	50	9	9
0.71534	0.05400	0.14502	50	10	10
0.33865	0.28466	0.14502	50	11	11
0.94600	0.66135	0.14502	50	12	12
0.00492	0.38702	0.81203	50	13	13
0.61298	0.61791	0.81203	50	14	14
0.38209	0.99508	0.81203	50	15	15
0.95141	0.27916	0.02146	50	16	16
0.32776	0.04859	0.02146	50	17	17
0.72084	0.67224	0.02146	50	18	18
0.32776	0.27916	0.02146	50	19	19
0.72084	0.04859	0.02146	50	20	20
0.95141	0.67224	0.02146	50	21	21
0.38209	0.38702	0.81203	50	22	22
0.00492	0.61791	0.81203	50	23	23
0.61298	0.99508	0.81203	50	24	24
0.67224	0.72084	0.97854	50	25	25
0.27916	0.95141	0.97854	50	26	26
0.04859	0.32776	0.97854	50	27	27
0.61791	0.61298	0.18797	50	28	28
0.99508	0.38209	0.18797	50	29	29
0.38702	0.00492	0.18797	50	30	30
0.99508	0.61298	0.18797	50	31	31
0.38702	0.38209	0.18797	50	32	32
0.61791	0.00492	0.18797	50	33	33
0.04859	0.72084	0.97854	50	34	34
0.67224	0.95141	0.97854	50	35	35

0.27916	0.32776	0.97854	50	36	36
0.54119	0.45881	0.04431	50	37	37
0.54119	0.08239	0.04431	50	38	38
0.91761	0.45881	0.04431	50	39	39
0.08239	0.54119	0.95569	50	40	40
0.45881	0.91761	0.95569	50	41	41
0.45881	0.54119	0.95569	50	42	42
0.20780	0.79220	0.21105	50	43	43
0.20780	0.41560	0.21105	50	44	44
0.58440	0.79220	0.21105	50	45	45
0.74926	0.87463	0.12216	50	46	46
0.12537	0.25074	0.12216	50	47	47
0.12537	0.87463	0.12216	50	48	48
0.87463	0.12537	0.87784	50	49	49
0.87463	0.74926	0.87784	50	50	50
0.25074	0.12537	0.87784	50	51	51
0.41560	0.20780	0.78895	50	52	52
0.79220	0.58440	0.78895	50	53	53
0.79220	0.20780	0.78895	50	54	54
0.00000	0.00000	0.06239	50	55	55
0.00000	0.00000	0.93761	50	56	56
0.66667	0.33333	0.22778	50	57	57
0.66667	0.33333	0.10411	50	58	58
0.33333	0.66667	0.89589	50	59	59
0.33333	0.66667	0.77222	50	60	60
0.54366	0.45634	0.11954	50	61	61
0.54366	0.08731	0.11954	50	62	62
0.91268	0.45634	0.11954	50	63	63
0.08731	0.54366	0.88045	50	64	64
0.45634	0.91268	0.88045	50	65	65
0.45634	0.54366	0.88045	50	66	66
0.20976	0.79024	0.78666	50	67	67
0.20976	0.41951	0.78666	50	68	68
0.58049	0.79024	0.78666	50	69	69
0.75402	0.87701	0.04699	50	70	70
0.12299	0.24598	0.04699	50	71	71
0.12299	0.87701	0.04699	50	72	72
0.87701	0.12299	0.95301	50	73	73
0.87701	0.75402	0.95301	50	74	74
0.24598	0.12299	0.95301	50	75	75
0.41951	0.20976	0.21334	50	76	76
0.79024	0.58049	0.21334	50	77	77
0.79024	0.20976	0.21334	50	78	78
0.00000	0.00000	0.10800	50	79	79
0.00000	0.00000	0.89200	50	80	80
0.66667	0.33333	0.77518	50	81	81
0.66667	0.33333	0.05849	50	82	82
0.33333	0.66667	0.94151	50	83	83
0.33333	0.66667	0.22482	50	84	84
0.46511	0.53489	0.08246	50	85	85

0.46511	0.93022	0.08246	50	86	86
0.06978	0.53489	0.08246	50	87	87
0.93022	0.46511	0.91754	50	88	88
0.53489	0.06978	0.91754	50	89	89
0.53489	0.46511	0.91754	50	90	90
0.13189	0.86811	0.24930	50	91	91
0.13189	0.26378	0.24930	50	92	92
0.73622	0.86811	0.24930	50	93	93
0.59695	0.79847	0.08405	50	94	94
0.20153	0.40305	0.08405	50	95	95
0.20153	0.79847	0.08405	50	96	96
0.79847	0.20153	0.91595	50	97	97
0.79847	0.59695	0.91595	50	98	98
0.40305	0.20153	0.91595	50	99	99
0.26378	0.13189	0.75070	50	100	100
0.86811	0.73622	0.75070	50	101	101
0.86811	0.13189	0.75070	50	102	102
0.00411	0.38075	0.31748	50	103	103
0.61925	0.62335	0.31748	50	104	104
0.37665	0.99589	0.31748	50	105	105
0.37665	0.38075	0.31748	50	106	106
0.00411	0.62335	0.31748	50	107	107
0.61925	0.99589	0.31748	50	108	108
0.41340	0.20670	0.28932	50	109	109
0.79330	0.58660	0.28932	50	110	110
0.79330	0.20670	0.28932	50	111	111
0.33333	0.66667	0.27051	50	112	112
0.20793	0.79207	0.28760	50	113	113
0.20793	0.41586	0.28760	50	114	114
0.58414	0.79207	0.28760	50	115	115
0.66667	0.33333	0.27322	50	116	116
0.26395	0.13198	0.25060	50	117	117
0.86802	0.73604	0.25060	50	118	118
0.86802	0.13198	0.25060	50	119	119
0.62335	0.61925	0.68252	50	120	120
0.99589	0.37665	0.68252	50	121	121
0.38075	0.00411	0.68252	50	122	122
0.99589	0.61925	0.68252	50	123	123
0.38075	0.37665	0.68252	50	124	124
0.62335	0.00411	0.68252	50	125	125
0.20670	0.79330	0.71068	50	126	126
0.20670	0.41340	0.71068	50	127	127
0.58660	0.79330	0.71068	50	128	128
0.66667	0.33333	0.72949	50	129	129
0.41586	0.20793	0.71240	50	130	130
0.79207	0.58414	0.71240	50	131	131
0.79207	0.20793	0.71240	50	132	132
0.33333	0.66667	0.72678	50	133	133
0.13198	0.86802	0.74940	50	134	134
0.13198	0.26395	0.74940	50	135	135

0.73604	0.86802	0.74940	50	136	136
0.50005	0.49995	0.72624	50	137	137
0.99990	0.49995	0.72624	50	138	138
0.50005	0.00010	0.72624	50	139	139
0.49995	0.50005	0.27376	50	140	140
0.00010	0.50005	0.27376	50	141	141
0.49995	0.99990	0.27376	50	142	142

S9.2 Germanium-Slab xyz Files

S9.2.1 Ge.db-monolayer (oP10)

$\rho = 0.1884\ \text{Å}^{-2} = 1.359\ \text{ML},\ E - E_{\text{bulk}} = 308\ \text{meV/at.}$

7.84310	0.00000	0.00000			
0.00000	38.86961	0.00000			
0.00000	0.00000	6.76570			
10 atoms					
0.02034	0.00000	0.81941	32	1	1
0.47966	0.00000	0.81941	32	2	2
0.52034	0.00000	0.18059	32	3	3
0.97966	0.00000	0.18059	32	4	4
0.25000	0.03815	0.67495	32	5	5
0.25000	0.96185	0.67495	32	6	6
0.75000	0.96185	0.32505	32	7	7
0.75000	0.03815	0.32505	32	8	8
0.25000	0.00000	0.37240	32	9	9
0.75000	0.00000	0.62760	32	10	10

S9.2.2 Ge.iso-II-2.5

$\rho = 0.3534\ \text{Å}^{-2} = 2.548\ \text{ML},\ E - E_{\text{bulk}} = 251\ \text{meV/at.}$

15.67423	0.00000	0.00000			
0.00000	11.19385	0.00000			
0.00000	0.00000	28.11850			
62 atoms					
0.00001	0.00000	0.00000	32	1	1
0.36467	0.00000	0.10991	32	2	2
0.36467	0.00000	0.89009	32	3	3
0.50130	0.00000	0.15808	32	4	4
0.50130	0.00000	0.84192	32	5	5
0.76010	0.00000	0.04475	32	6	6
0.76010	0.00000	0.95525	32	7	7
0.91225	0.00000	0.07406	32	8	8
0.91225	0.00000	0.92595	32	9	9
0.49329	0.00000	0.05356	32	10	10
0.49329	0.00000	0.94644	32	11	11
0.24297	0.11297	0.00000	32	12	12
0.24297	0.88703	0.00000	32	13	13
0.55267	0.16644	0.10305	32	14	14
0.55267	0.83356	0.89694	32	15	15
0.55267	0.16644	0.89694	32	16	16
0.55267	0.83356	0.10305	32	17	17
0.30975	0.18824	0.07465	32	18	18
0.30975	0.81176	0.92535	32	19	19
0.30975	0.18824	0.92535	32	20	20

0.30975	0.81176	0.07465	32	21	21
0.95601	0.17575	0.12814	32	22	22
0.95601	0.82425	0.87186	32	23	23
0.95601	0.17575	0.87186	32	24	24
0.95601	0.82425	0.12814	32	25	25
0.08999	0.18182	0.00000	32	26	26
0.08999	0.81818	0.00000	32	27	27
0.69977	0.19543	0.07184	32	28	28
0.69977	0.80456	0.92816	32	29	29
0.69977	0.19543	0.92816	32	30	30
0.69977	0.80456	0.07184	32	31	31
0.05137	0.29872	0.07307	32	32	32
0.05137	0.70128	0.92693	32	33	33
0.05137	0.29872	0.92693	32	34	34
0.05137	0.70128	0.07307	32	35	35
0.66295	0.31657	0.00000	32	36	36
0.66295	0.68343	0.00000	32	37	37
0.83205	0.29264	0.10315	32	38	38
0.83205	0.70736	0.89685	32	39	39
0.83205	0.29264	0.89685	32	40	40
0.83205	0.70736	0.10315	32	41	41
0.44360	0.31369	0.07471	32	42	42
0.44360	0.68631	0.92529	32	43	43
0.44360	0.31369	0.92529	32	44	44
0.44360	0.68631	0.07471	32	45	45
0.19963	0.33467	0.10130	32	46	46
0.19963	0.66533	0.89870	32	47	47
0.19963	0.33467	0.89870	32	48	48
0.19963	0.66533	0.10130	32	49	49
0.51078	0.38706	0.00000	32	50	50
0.51078	0.61294	0.00000	32	51	51
0.25094	0.50000	0.15702	32	52	52
0.25094	0.50000	0.84298	32	53	53
0.26308	0.50000	0.05291	32	54	54
0.26308	0.50000	0.94709	32	55	55
0.38975	0.50000	0.11150	32	56	56
0.38975	0.50000	0.88850	32	57	57
0.75200	0.50000	0.00000	32	58	58
0.84553	0.50000	0.07091	32	59	59
0.84553	0.50000	0.92909	32	60	60
0.99777	0.50000	0.04467	32	61	61
0.99777	0.50000	0.95533	32	62	62

S9.2.3 Ge.equi-II-3

$\rho = 0.4037\ \text{Å}^{-2} = 2.911\ \text{ML},\ E - E_{\text{bulk}} = 222\ \text{meV/at.}$

10.88372	-0.00000	0.00204			
-5.44186	9.33195	-0.00089			
0.00667	0.00048	34.96546			
41 atoms					
0.33470	0.04609	0.25061	50	1	1
0.95527	0.28723	0.25061	50	2	2
0.72578	0.66666	0.24872	50	3	3
0.71201	0.04620	0.25327	50	4	4
0.33247	0.28712	0.25327	50	5	5
0.96033	0.66666	0.25513	50	6	6
0.92142	0.25204	0.07214	50	7	7
0.33606	0.08131	0.07214	50	8	8
0.74943	0.66668	0.07242	50	9	9
0.33610	0.29972	0.04765	50	10	10
0.70306	0.03364	0.04765	50	11	11
0.96650	0.66668	0.04764	50	12	12
0.53293	0.44755	0.09586	50	13	13
0.55305	0.08189	0.09515	50	14	14
0.91793	0.46807	0.09555	50	15	15
0.75604	0.87970	0.21275	50	16	16
0.12609	0.24659	0.21253	50	17	17
0.12317	0.87502	0.21254	50	18	18
0.00216	0.00060	0.11854	50	19	19
0.66819	0.33376	0.18882	50	20	20
0.54300	0.45362	0.21275	50	21	21
0.54616	0.08674	0.21253	50	22	22
0.91481	0.45831	0.21254	50	23	23
0.75205	0.88580	0.09586	50	24	24
0.13783	0.25146	0.09515	50	25	25
0.11654	0.86528	0.09555	50	26	26
0.00110	0.99957	0.18882	50	27	27
0.66823	0.33274	0.11854	50	28	28
0.46653	0.53371	0.15486	50	29	29
0.46666	0.92995	0.15442	50	30	30
0.06985	0.53440	0.15449	50	31	31
0.59949	0.79963	0.15486	50	32	32
0.20338	0.40338	0.15442	50	33	33
0.20212	0.79894	0.15449	50	34	34
0.12584	0.49295	0.29437	50	35	35
0.05444	0.66665	0.32424	50	36	36
0.32321	0.44254	0.30830	50	37	37
0.29955	0.84037	0.29437	50	38	38
0.55285	0.66666	0.29650	50	39	39
0.54732	0.89077	0.30830	50	40	40
0.36303	0.66666	0.24997	50	41	41

S9.2.4 Ge.equi-II-3.5

$\rho = 0.4781$ Å^{-2} $= 3.448$ ML, $E - E_{\text{bulk}} = 183$ meV/at.

10.71370 -0.01100 -0.00829
-5.49272 9.36400 -0.25389
-0.21007 -0.40637 30.60224
48 atoms

0.03938	0.81651	0.19581	32	1	1
0.04665	0.82625	0.27601	32	2	2
0.11219	0.35595	0.23590	32	3	3
0.13361	0.25074	0.05846	32	4	4
0.21634	0.29959	0.39743	32	5	5
0.18713	0.50189	0.07438	32	6	6
0.16572	0.49868	0.41335	32	7	7
0.15609	0.05849	0.16867	32	8	8
0.17348	0.07731	0.30260	32	9	9
0.16140	0.68985	0.16920	32	10	10
0.16828	0.70342	0.30314	32	11	11
0.24190	0.22156	0.23555	32	12	12
0.24199	0.62007	0.23625	32	13	13
0.36033	0.24629	0.07152	32	14	14
0.39287	0.23103	0.43153	32	15	15
0.35751	0.74388	0.04028	32	16	16
0.39007	0.72863	0.40028	32	17	17
0.36533	0.08255	0.12695	32	18	18
0.38570	0.12853	0.35199	32	19	19
0.36468	0.84638	0.11982	32	20	20
0.38505	0.89237	0.34486	32	21	21
0.50849	0.75334	0.23626	32	22	22
0.50840	0.35482	0.23555	32	23	23
0.98625	0.47286	0.12520	32	24	24
0.00594	0.49970	0.34986	32	25	25
0.98530	0.09568	0.12195	32	26	26
0.00628	0.12315	0.34661	32	27	27
0.95036	0.26790	0.16891	32	28	28
0.96249	0.28829	0.30290	32	29	29
0.78790	0.68665	0.16891	32	30	30
0.80003	0.70702	0.30290	32	31	31
0.74445	0.47524	0.12195	32	32	32
0.76413	0.50205	0.34661	32	33	33
0.74412	0.85179	0.12521	32	34	34
0.76510	0.87925	0.34986	32	35	35
0.70374	0.14867	0.19581	32	36	36
0.71101	0.15841	0.27601	32	37	37
0.63820	0.61894	0.23591	32	38	38
0.58467	0.47626	0.05846	32	39	39
0.56325	0.47301	0.39743	32	40	40
0.53406	0.67535	0.07439	32	41	41
0.61677	0.72416	0.41335	32	42	42
0.58211	0.27149	0.16866	32	43	43
0.58897	0.28505	0.30261	32	44	44

0.57690	0.89760	0.16922	32	45	45
0.59430	0.91642	0.30314	32	46	46
0.36517	0.44353	0.12499	32	47	47
0.38523	0.53138	0.34682	32	48	48

S9.2.5 Ge.iso-II-4

$\rho = 0.5461$ Å$^{-2} = 3.939$ ML, $E - E_{\mathrm{bulk}} = 176$ meV/at.

-15.82209	15.82209	0.00000			
-0.00007	-0.00007	15.71212			
47.38157	47.38157	-0.00043			
192 atoms					
0.00000	0.88780	0.12974	32	1	1
0.00000	0.50254	0.93508	32	2	2
0.94334	0.00665	0.08217	32	3	3
0.94333	0.24350	0.00107	32	4	4
0.89604	0.92204	0.95858	32	5	5
0.90596	0.94148	0.05038	32	6	6
0.90724	0.94027	0.11385	32	7	7
0.90850	0.09119	0.00154	32	8	8
0.90851	0.15890	0.08174	32	9	9
0.90729	0.30984	0.96935	32	10	10
0.90595	0.30842	0.03291	32	11	11
0.89610	0.32794	0.12476	32	12	12
0.89967	0.70122	0.97045	32	13	13
0.90120	0.69291	0.03171	32	14	14
0.91681	0.69646	0.12495	32	15	15
0.91682	0.55370	0.95830	32	16	16
0.90118	0.55689	0.05163	32	17	17
0.89971	0.54879	0.11290	32	18	18
0.84765	0.05524	0.97125	32	19	19
0.84821	0.05655	0.03191	32	20	20
0.83387	0.04919	0.12574	32	21	21
0.83387	0.20091	0.95740	32	22	22
0.84819	0.19337	0.05138	32	23	23
0.84772	0.19496	0.11203	32	24	24
0.83869	0.79897	0.94772	32	25	25
0.84356	0.80720	0.05037	32	26	26
0.84406	0.80743	0.11390	32	27	27
0.84113	0.66051	0.00105	32	28	28
0.84112	0.58926	0.08229	32	29	29
0.84409	0.44269	0.96935	32	30	30
0.84354	0.44266	0.03297	32	31	31
0.83878	0.45095	0.13564	32	32	32
0.80668	0.74184	0.08225	32	33	33
0.80669	0.50793	0.00105	32	34	34
0.75000	0.99383	0.98263	32	35	35

0.75000	0.99488	0.02032	32	36	36
0.75000	0.99855	0.14880	32	37	37
0.74999	0.84154	0.97019	32	38	38
0.75000	0.84207	0.03112	32	39	39
0.75000	0.86023	0.12929	32	40	40
0.75000	0.75066	0.00081	32	41	41
0.75000	0.49909	0.08258	32	42	42
0.75000	0.25199	0.93431	32	43	43
0.75000	0.25501	0.06302	32	44	44
0.75000	0.25613	0.10069	32	45	45
0.75000	0.39037	0.95384	32	46	46
0.75000	0.40784	0.05223	32	47	47
0.75000	0.40835	0.11322	32	48	48
0.69332	0.74184	0.08225	32	49	49
0.69331	0.50793	0.00106	32	50	50
0.66129	0.79900	0.94773	32	51	51
0.65644	0.80720	0.05037	32	52	52
0.65594	0.80743	0.11390	32	53	53
0.65888	0.66051	0.00106	32	54	54
0.65889	0.58926	0.08229	32	55	55
0.65592	0.44270	0.96935	32	56	56
0.65647	0.44266	0.03297	32	57	57
0.66123	0.45096	0.13564	32	58	58
0.65235	0.05525	0.97125	32	59	59
0.65179	0.05655	0.03191	32	60	60
0.66613	0.04919	0.12574	32	61	61
0.66614	0.20092	0.95740	32	62	62
0.65181	0.19337	0.05138	32	63	63
0.65228	0.19496	0.11203	32	64	64
0.60032	0.70122	0.97045	32	65	65
0.59880	0.69291	0.03172	32	66	66
0.58319	0.69646	0.12495	32	67	67
0.58319	0.55371	0.95829	32	68	68
0.59883	0.55689	0.05163	32	69	69
0.60030	0.54879	0.11290	32	70	70
0.60393	0.92205	0.95860	32	71	71
0.59404	0.94148	0.05038	32	72	72
0.59276	0.94027	0.11385	32	73	73
0.59150	0.09119	0.00154	32	74	74
0.59149	0.15890	0.08174	32	75	75
0.59271	0.30985	0.96935	32	76	76
0.59405	0.30842	0.03291	32	77	77
0.60390	0.32794	0.12476	32	78	78
0.55666	0.00665	0.08217	32	79	79
0.55667	0.24350	0.00107	32	80	80
0.49998	0.90791	0.97172	32	81	81
0.50000	0.90693	0.03132	32	82	82
0.50000	0.88780	0.12974	32	83	83
0.50000	0.75359	0.02030	32	84	84
0.50000	0.00101	0.00159	32	85	85

0.50000	0.24902	0.08172	32	86	86
0.50001	0.36206	0.95334	32	87	87
0.50000	0.34292	0.05197	32	88	88
0.50000	0.49621	0.06306	32	89	89
0.50000	0.49435	0.10075	32	90	90
0.99998	0.90791	0.97172	32	91	91
0.00000	0.90693	0.03132	32	92	92
0.99999	0.75551	0.98260	32	93	93
1.00000	0.75359	0.02030	32	94	94
1.00000	0.74775	0.14810	32	95	95
1.00000	0.00101	0.00159	32	96	96
0.00000	0.24902	0.08172	32	97	97
0.00000	0.36206	0.95334	32	98	98
0.00000	0.34292	0.05197	32	99	99
0.00000	0.34197	0.11162	32	100	100
0.00000	0.49621	0.06306	32	101	101
0.00000	0.49435	0.10075	32	102	102
0.05666	0.00665	0.08217	32	103	103
0.05667	0.24350	0.00107	32	104	104
0.10393	0.92205	0.95860	32	105	105
0.09404	0.94148	0.05038	32	106	106
0.09276	0.94027	0.11385	32	107	107
0.09150	0.09119	0.00154	32	108	108
0.09150	0.15890	0.08174	32	109	109
0.09272	0.30985	0.96935	32	110	110
0.09406	0.30842	0.03291	32	111	111
0.10390	0.32794	0.12476	32	112	112
0.10032	0.70122	0.97045	32	113	113
0.09880	0.69291	0.03172	32	114	114
0.08319	0.69646	0.12495	32	115	115
0.08319	0.55371	0.95829	32	116	116
0.09883	0.55689	0.05163	32	117	117
0.10030	0.54879	0.11290	32	118	118
0.15235	0.05525	0.97125	32	119	119
0.15179	0.05655	0.03191	32	120	120
0.16613	0.04919	0.12574	32	121	121
0.16614	0.20092	0.95740	32	122	122
0.15181	0.19337	0.05138	32	123	123
0.15228	0.19496	0.11203	32	124	124
0.16129	0.79900	0.94773	32	125	125
0.15644	0.80720	0.05037	32	126	126
0.15594	0.80743	0.11390	32	127	127
0.15888	0.66051	0.00106	32	128	128
0.15888	0.58926	0.08229	32	129	129
0.15592	0.44270	0.96935	32	130	130
0.15647	0.44266	0.03297	32	131	131
0.16123	0.45096	0.13564	32	132	132
0.19332	0.74184	0.08225	32	133	133
0.19331	0.50793	0.00106	32	134	134
0.25000	0.99383	0.98263	32	135	135

0.25000	0.99488	0.02032	32	136	136
0.25000	0.99855	0.14880	32	137	137
0.24999	0.84154	0.97019	32	138	138
0.25000	0.84207	0.03112	32	139	139
0.25000	0.86023	0.12929	32	140	140
0.25000	0.75066	0.00081	32	141	141
0.25000	0.49909	0.08258	32	142	142
0.25000	0.25199	0.93431	32	143	143
0.25000	0.25501	0.06302	32	144	144
0.25000	0.25613	0.10069	32	145	145
0.25000	0.39037	0.95384	32	146	146
0.25000	0.40784	0.05223	32	147	147
0.25000	0.40835	0.11322	32	148	148
0.30668	0.74184	0.08225	32	149	149
0.30669	0.50793	0.00105	32	150	150
0.33869	0.79897	0.94772	32	151	151
0.34356	0.80720	0.05037	32	152	152
0.34406	0.80743	0.11390	32	153	153
0.34113	0.66051	0.00105	32	154	154
0.34112	0.58926	0.08229	32	155	155
0.34409	0.44269	0.96935	32	156	156
0.34354	0.44266	0.03297	32	157	157
0.33877	0.45095	0.13564	32	158	158
0.34765	0.05524	0.97125	32	159	159
0.34821	0.05655	0.03191	32	160	160
0.33387	0.04919	0.12574	32	161	161
0.33387	0.20091	0.95740	32	162	162
0.34819	0.19337	0.05138	32	163	163
0.34772	0.19496	0.11203	32	164	164
0.39967	0.70122	0.97045	32	165	165
0.40120	0.69291	0.03171	32	166	166
0.41681	0.69646	0.12495	32	167	167
0.41682	0.55370	0.95830	32	168	168
0.40118	0.55689	0.05163	32	169	169
0.39971	0.54879	0.11290	32	170	170
0.39604	0.92204	0.95858	32	171	171
0.40596	0.94148	0.05038	32	172	172
0.40724	0.94027	0.11385	32	173	173
0.40849	0.09119	0.00154	32	174	174
0.40851	0.15890	0.08174	32	175	175
0.40729	0.30984	0.96935	32	176	176
0.40595	0.30842	0.03291	32	177	177
0.39610	0.32794	0.12476	32	178	178
0.44334	0.00665	0.08217	32	179	179
0.44333	0.24350	0.00107	32	180	180
0.50000	0.75551	0.98260	32	181	181
0.50000	0.74775	0.14810	32	182	182
0.50000	0.34197	0.11162	32	183	183
0.50000	0.50254	0.93508	32	184	184

0.00001	0.48841	0.97807	32	185	185
0.75000	0.26178	0.97745	32	186	186
0.25000	0.26178	0.97745	32	187	187
0.50001	0.48841	0.97807	32	188	188
0.75000	0.98864	0.10562	32	189	189
1.00000	0.76126	0.10506	32	190	190
0.25000	0.98864	0.10562	32	191	191
0.50000	0.76126	0.10506	32	192	192

S9.2.6 Ge.equi-II-6

$\rho = 0.8042$ Å^{-2} $= 5.800$ ML, $E - E_{\mathrm{bulk}} = 120$ meV/at.

10.86109	-0.01836	-0.00140			
-5.44644	9.39675	-0.00201			
-0.00506	-0.01138	38.26388			
82 atoms					
0.34308	0.99782	0.20027	32	1	1
0.95338	0.22993	0.20030	32	2	2
0.72149	0.60798	0.20028	32	3	3
0.72123	0.99788	0.20033	32	4	4
0.34308	0.22938	0.20035	32	5	5
0.95299	0.60771	0.20028	32	6	6
0.96265	0.23156	0.02246	32	7	7
0.33972	0.98994	0.02231	32	8	8
0.71411	0.61309	0.02088	32	9	9
0.33792	0.23100	0.02467	32	10	10
0.71970	0.99048	0.02487	32	11	11
0.94899	0.61236	0.02657	32	12	12
0.62392	0.55966	0.26098	32	13	13
0.00197	0.32778	0.26100	32	14	14
0.39179	0.94936	0.26101	32	15	15
0.00168	0.55928	0.26101	32	16	16
0.39187	0.32751	0.26096	32	17	17
0.62336	0.94936	0.26094	32	18	18
0.55050	0.40345	0.05898	32	19	19
0.54819	0.03198	0.05903	32	20	20
0.91888	0.39903	0.05877	32	21	21
0.21366	0.73739	0.29415	32	22	22
0.21406	0.36150	0.29395	32	23	23
0.59000	0.73776	0.29395	32	24	24
0.75507	0.81993	0.16734	32	25	25
0.13133	0.19586	0.16734	32	26	26
0.13097	0.81953	0.16713	32	27	27
0.00616	0.94435	0.08239	32	28	28
0.67271	0.27901	0.31721	32	29	29
0.67247	0.27846	0.14409	32	30	30
0.54885	0.40170	0.16467	32	31	31
0.54892	0.03090	0.16469	32	32	32

0.92028	0.40228	0.16462	32	33	33
0.75975	0.82036	0.06012	32	34	34
0.12706	0.18979	0.06017	32	35	35
0.13048	0.82432	0.05992	32	36	36
0.42506	0.15537	0.29660	32	37	37
0.79642	0.52673	0.29667	32	38	38
0.79584	0.15530	0.29662	32	39	39
0.00578	0.94493	0.14701	32	40	40
0.67283	0.27877	0.08011	32	41	41
0.33916	0.61231	0.31428	32	42	42
0.47142	0.47972	0.11194	32	43	43
0.47075	0.87492	0.11187	32	44	44
0.07566	0.47956	0.11171	32	45	45
0.13824	0.81366	0.34849	32	46	46
0.13788	0.21000	0.34825	32	47	47
0.74200	0.81360	0.34828	32	48	48
0.60333	0.74352	0.11303	32	49	49
0.20693	0.34763	0.11302	32	50	50
0.20700	0.74388	0.11280	32	51	51
0.00788	0.32120	0.44041	32	52	52
0.62631	0.56969	0.43883	32	53	53
0.38469	0.94679	0.43897	32	54	54
0.38521	0.32675	0.43642	32	55	55
0.00710	0.55604	0.43472	32	56	56
0.62574	0.94497	0.43662	32	57	57
0.42658	0.15510	0.40225	32	58	58
0.79363	0.52576	0.40252	32	59	59
0.79807	0.15739	0.40231	32	60	60
0.33886	0.61299	0.37890	32	61	61
0.21890	0.73738	0.40136	32	62	62
0.21495	0.36666	0.40117	32	63	63
0.58439	0.73396	0.40112	32	64	64
0.67328	0.27961	0.38118	32	65	65
0.26929	0.07742	0.34942	32	66	66
0.87392	0.68234	0.34958	32	67	67
0.87409	0.07810	0.34935	32	68	68
0.12613	0.38780	0.97224	32	69	69
0.12048	0.61134	0.98264	32	70	70
0.37306	0.43569	0.98467	32	71	71
0.34993	0.83480	0.97218	32	72	72
0.61879	0.61212	0.95792	32	73	73
0.54857	0.78605	0.98497	32	74	74
0.78277	0.73339	0.48905	32	75	75
0.83059	0.98027	0.47662	32	76	76
0.00628	0.72773	0.47865	32	77	77
0.00715	0.22614	0.50337	32	78	78
0.22977	0.95724	0.48911	32	79	79
0.18093	0.15579	0.47631	32	80	80
0.31126	0.61126	0.02520	32	81	81
0.00596	0.91831	0.43609	32	82	82

S9.3 Silicon-Slab xyz Files

S9.3.1 Si.db-monolayer (oP10)

$\rho = 0.2110\ \text{Å}^{-2} = 1.364\ \text{ML},\ E - E_{\text{bulk}} = 430\ \text{meV/at.}$

```
7.40937     0.00000     0.00000
0.00000     35.75410    0.00000
0.00000     0.00000     6.39543
10 atoms
0.01913     0.00000     0.81934     14    1     1
0.48087     0.00000     0.81934     14    2     2
0.51913     0.00000     0.18066     14    3     3
0.98087     0.00000     0.18066     14    4     4
0.25000     0.03788     0.67701     14    5     5
0.25000     0.96212     0.67701     14    6     6
0.75000     0.96212     0.32299     14    7     7
0.75000     0.03788     0.32299     14    8     8
0.25000     0.00000     0.37407     14    9     9
0.75000     0.00000     0.62593     14    10    10
```

S9.3.2 Si.iso-II-2.5

$\rho = 0.3851\ \text{Å}^{-2} = 2.489\ \text{ML},\ E - E_{\text{bulk}} = 322\ \text{meV/at.}$

```
15.01360    0.00000     0.00000
0.00000     10.72374    0.00000
0.00000     0.00000     24.81168
62 atoms
0.00530     0.00000     0.00000     14    1     1
0.36693     0.00000     0.11410     14    2     2
0.36693     0.00000     0.88590     14    3     3
0.50034     0.00000     0.16477     14    4     4
0.50034     0.00000     0.83523     14    5     5
0.76091     0.00000     0.04838     14    6     6
0.76091     0.00000     0.95162     14    7     7
0.91223     0.00000     0.07669     14    8     8
0.91223     0.00000     0.92331     14    9     9
0.49346     0.00000     0.05520     14    10    10
0.49346     0.00000     0.94480     14    11    11
0.24599     0.11233     0.00000     14    12    12
0.24599     0.88767     0.00000     14    13    13
0.55251     0.16366     0.10837     14    14    14
0.55251     0.83634     0.89163     14    15    15
0.55251     0.16366     0.89163     14    16    16
0.55251     0.83634     0.10837     14    17    17
0.31244     0.18904     0.07990     14    18    18
0.31244     0.81096     0.92010     14    19    19
0.31244     0.18904     0.92010     14    20    20
```

0.31244	0.81096	0.07990	14	21	21
0.94147	0.19531	0.11305	14	22	22
0.94147	0.80469	0.88695	14	23	23
0.94147	0.19531	0.88695	14	24	24
0.94147	0.80469	0.11305	14	25	25
0.09512	0.18183	0.00000	14	26	26
0.09512	0.81817	0.00000	14	27	27
0.69757	0.19292	0.07633	14	28	28
0.69757	0.80708	0.92367	14	29	29
0.69757	0.19292	0.92367	14	30	30
0.69757	0.80708	0.07633	14	31	31
0.06053	0.30706	0.07633	14	32	32
0.06053	0.69294	0.92367	14	33	33
0.06053	0.30706	0.92367	14	34	34
0.06053	0.69294	0.07633	14	35	35
0.66301	0.31816	0.00000	14	36	36
0.66301	0.68185	0.00000	14	37	37
0.81674	0.30459	0.11295	14	38	38
0.81674	0.69541	0.88705	14	39	39
0.81674	0.30459	0.88705	14	40	40
0.81674	0.69541	0.11295	14	41	41
0.44568	0.31096	0.07990	14	42	42
0.44568	0.68904	0.92010	14	43	43
0.44568	0.31096	0.92010	14	44	44
0.44568	0.68904	0.07990	14	45	45
0.20560	0.33635	0.10836	14	46	46
0.20560	0.66365	0.89164	14	47	47
0.20560	0.33635	0.89164	14	48	48
0.20560	0.66365	0.10836	14	49	49
0.51214	0.38767	0.00000	14	50	50
0.51214	0.61233	0.00000	14	51	51
0.25778	0.50000	0.16477	14	52	52
0.25778	0.50000	0.83523	14	53	53
0.26467	0.50000	0.05519	14	54	54
0.26467	0.50000	0.94481	14	55	55
0.39120	0.50000	0.11411	14	56	56
0.39120	0.50000	0.88589	14	57	57
0.75282	0.50000	0.00000	14	58	58
0.84591	0.50000	0.07668	14	59	59
0.84591	0.50000	0.92332	14	60	60
0.99722	0.50000	0.04837	14	61	61
0.99722	0.50000	0.95163	14	62	62

S9.3.3 Si.equi-II-3

$\rho = 0.5032\ \text{Å}^{-2} = 3.253\ \text{ML},\ E - E_{\text{bulk}} = 280\ \text{meV/at.}$

10.27433 -0.00034 0.00000
-5.13746 8.89766 -0.00000
0.00001 -0.00000 26.09222
46 atoms

0.33334	0.04309	0.27406	14	1	1
0.95693	0.29027	0.27407	14	2	2
0.70976	0.66667	0.27406	14	3	3
0.71884	0.05218	0.27250	14	4	4
0.33333	0.28116	0.27251	14	5	5
0.94782	0.66666	0.27251	14	6	6
0.95693	0.29027	0.02445	14	7	7
0.33334	0.04309	0.02445	14	8	8
0.70976	0.66667	0.02445	14	9	9
0.33333	0.28116	0.02601	14	10	10
0.71884	0.05218	0.02601	14	11	11
0.94782	0.66666	0.02601	14	12	12
0.54259	0.45614	0.07488	14	13	13
0.54385	0.08644	0.07488	14	14	14
0.91356	0.45741	0.07488	14	15	15
0.75311	0.87719	0.22364	14	16	16
0.12407	0.24689	0.22364	14	17	17
0.12280	0.87592	0.22363	14	18	18
0.00001	0.00000	0.10469	14	19	19
0.66667	0.33334	0.19382	14	20	20
0.54259	0.45614	0.22363	14	21	21
0.54386	0.08644	0.22364	14	22	22
0.91356	0.45741	0.22364	14	23	23
0.75311	0.87718	0.07488	14	24	24
0.12407	0.24689	0.07488	14	25	25
0.12281	0.87593	0.07488	14	26	26
0.00001	0.00000	0.19382	14	27	27
0.66667	0.33334	0.10469	14	28	28
0.46565	0.53450	0.14926	14	29	29
0.46550	0.93115	0.14926	14	30	30
0.06885	0.53434	0.14926	14	31	31
0.59782	0.79884	0.14926	14	32	32
0.20101	0.40218	0.14926	14	33	33
0.20117	0.79898	0.14926	14	34	34
0.10121	0.43454	0.34567	14	35	35
0.13149	0.66665	0.32727	14	36	36
0.33332	0.46483	0.32727	14	37	37
0.33333	0.89878	0.34565	14	38	38
0.56544	0.66667	0.34565	14	39	39
0.53517	0.86850	0.32727	14	40	40
0.10121	0.43454	0.95284	14	41	41
0.13150	0.66665	0.97125	14	42	42
0.33332	0.46483	0.97125	14	43	43
0.33333	0.89878	0.95286	14	44	44
0.56544	0.66667	0.95286	14	45	45
0.53517	0.86850	0.97125	14	46	46

S9.3.4 Si.iso-II-4
$\rho = 0.6056$ Å$^{-2} = 3.915$ ML, $E - E_{\mathrm{bulk}} = 232$ meV/at.

10.62542	0.00000	0.00000			
0.00000	14.91779	0.00000			
0.00000	0.00000	34.35054			
96 atoms					
0.25000	0.51535	0.23141	14	1	1
0.75000	0.48465	0.23141	14	2	2
0.25000	0.11281	0.95396	14	3	3
0.75000	0.88719	0.95396	14	4	4
0.25000	0.12141	0.87777	14	5	5
0.75000	0.87859	0.87777	14	6	6
0.13684	0.63142	0.14602	14	7	7
0.86316	0.36858	0.14602	14	8	8
0.36316	0.63142	0.14602	14	9	9
0.63684	0.36858	0.14602	14	10	10
0.13684	0.86858	0.99724	14	11	11
0.86316	0.13142	0.99724	14	12	12
0.36316	0.86858	0.99724	14	13	13
0.63684	0.13142	0.99724	14	14	14
0.05522	0.56261	0.91432	14	15	15
0.94478	0.43739	0.91432	14	16	16
0.44478	0.56261	0.91432	14	17	17
0.55522	0.43739	0.91432	14	18	18
0.06192	0.56696	0.08724	14	19	19
0.93808	0.43304	0.08724	14	20	20
0.43808	0.56696	0.08724	14	21	21
0.56192	0.43304	0.08724	14	22	22
0.06162	0.56646	0.20451	14	23	23
0.93838	0.43354	0.20451	14	24	24
0.43838	0.56646	0.20451	14	25	25
0.56162	0.43354	0.20451	14	26	26
0.06764	0.71671	0.99726	14	27	27
0.93236	0.28329	0.99726	14	28	28
0.43236	0.71671	0.99726	14	29	29
0.56764	0.28329	0.99726	14	30	30
0.06763	0.78329	0.14600	14	31	31
0.93237	0.21671	0.14600	14	32	32
0.43237	0.78329	0.14600	14	33	33
0.56763	0.21671	0.14600	14	34	34
0.06161	0.93353	0.93876	14	35	35
0.93839	0.06647	0.93876	14	36	36
0.43839	0.93353	0.93876	14	37	37
0.56161	0.06647	0.93876	14	38	38
0.06191	0.93304	0.05602	14	39	39
0.93809	0.06696	0.05602	14	40	40

0.43809	0.93304	0.05602	14	41	41
0.56191	0.06696	0.05602	14	42	42
0.05523	0.93739	0.22893	14	43	43
0.94477	0.06261	0.22893	14	44	44
0.44477	0.93739	0.22893	14	45	45
0.55523	0.06261	0.22893	14	46	46
0.05633	0.31849	0.94166	14	47	47
0.94367	0.68151	0.94166	14	48	48
0.44367	0.31849	0.94166	14	49	49
0.55633	0.68151	0.94166	14	50	50
0.05362	0.31807	0.05335	14	51	51
0.94638	0.68193	0.05335	14	52	52
0.44638	0.31807	0.05335	14	53	53
0.55362	0.68193	0.05335	14	54	54
0.08304	0.32564	0.22620	14	55	55
0.91696	0.67436	0.22620	14	56	56
0.41696	0.32564	0.22620	14	57	57
0.58304	0.67436	0.22620	14	58	58
0.08305	0.17437	0.91707	14	59	59
0.91695	0.82563	0.91707	14	60	60
0.41695	0.17437	0.91707	14	61	61
0.58305	0.82563	0.91707	14	62	62
0.05362	0.18193	0.08991	14	63	63
0.94638	0.81807	0.08991	14	64	64
0.44638	0.18193	0.08991	14	65	65
0.55362	0.81807	0.08991	14	66	66
0.05633	0.18151	0.20160	14	67	67
0.94367	0.81849	0.20160	14	68	68
0.44367	0.18151	0.20160	14	69	69
0.55633	0.81849	0.20160	14	70	70
0.25000	0.38114	0.96221	14	71	71
0.75000	0.61886	0.96221	14	72	72
0.25000	0.37950	0.03194	14	73	73
0.75000	0.62050	0.03194	14	74	74
0.25000	0.38720	0.18930	14	75	75
0.75000	0.61280	0.18930	14	76	76
0.25000	0.37859	0.26550	14	77	77
0.75000	0.62141	0.26550	14	78	78
0.25000	0.53273	0.94144	14	79	79
0.75000	0.46727	0.94144	14	80	80
0.25000	0.53248	0.05212	14	81	81
0.75000	0.46752	0.05212	14	82	82
0.25000	0.62605	0.99685	14	83	83
0.75000	0.37395	0.99685	14	84	84
0.25000	0.87395	0.14640	14	85	85
0.75000	0.12605	0.14640	14	86	86
0.25000	0.12050	0.11132	14	87	87
0.75000	0.87950	0.11132	14	88	88
0.25000	0.11887	0.18105	14	89	89

0.75000	0.88113	0.18105	14	90	90
0.25000	0.98466	0.91187	14	91	91
0.75000	0.01534	0.91187	14	92	92
0.25000	0.96752	0.09113	14	93	93
0.75000	0.03248	0.09113	14	94	94
0.25000	0.96728	0.20182	14	95	95
0.75000	0.03272	0.20182	14	96	96

S9.3.5 Si.iso-II-5

$\rho = 0.8272\ \text{Å}^{-2} = 5.347\ \text{ML},\ E - E_{\text{bulk}} = 186\ \text{meV/at.}$

10.57224	0.00000	0.00000			
0.00000	14.86573	0.00000			
0.00000	0.00000	43.59367			
130 atoms					
0.25000	0.62159	0.21259	14	1	1
0.25000	0.62159	0.78741	14	2	2
0.75000	0.37841	0.78741	14	3	3
0.75000	0.37841	0.21259	14	4	4
0.25000	0.48433	0.18583	14	5	5
0.25000	0.48433	0.81417	14	6	6
0.75000	0.51567	0.81417	14	7	7
0.75000	0.51567	0.18583	14	8	8
0.25000	0.61260	0.15253	14	9	9
0.25000	0.61260	0.84747	14	10	10
0.75000	0.38740	0.84747	14	11	11
0.75000	0.38740	0.15253	14	12	12
0.25000	0.03275	0.83797	14	13	13
0.25000	0.03275	0.16203	14	14	14
0.75000	0.96725	0.16203	14	15	15
0.75000	0.96725	0.83797	14	16	16
0.63655	0.63102	0.11807	14	17	17
0.86345	0.63102	0.88193	14	18	18
0.13655	0.36898	0.88193	14	19	19
0.36345	0.36898	0.11807	14	20	20
0.36345	0.36898	0.88193	14	21	21
0.13655	0.36898	0.11807	14	22	22
0.86345	0.63102	0.11807	14	23	23
0.63655	0.63102	0.88193	14	24	24
0.63592	0.86935	0.00000	14	25	25
0.86408	0.86935	0.00000	14	26	26
0.13592	0.13065	0.00000	14	27	27
0.36408	0.13065	0.00000	14	28	28
0.58265	0.32544	0.18156	14	29	29
0.91735	0.32544	0.81844	14	30	30
0.08265	0.67456	0.81844	14	31	31
0.41735	0.67456	0.18156	14	32	32

0.41735	0.67456	0.81844	14	33	33
0.08265	0.67456	0.18156	14	34	34
0.91735	0.32544	0.18156	14	35	35
0.58265	0.32544	0.81844	14	36	36
0.56182	0.56654	0.16429	14	37	37
0.93818	0.56654	0.83571	14	38	38
0.06182	0.43346	0.83571	14	39	39
0.43818	0.43346	0.16429	14	40	40
0.43818	0.43346	0.83571	14	41	41
0.06182	0.43346	0.16429	14	42	42
0.93818	0.56654	0.16429	14	43	43
0.56182	0.56654	0.83571	14	44	44
0.55537	0.93719	0.18366	14	45	45
0.94463	0.93719	0.81634	14	46	46
0.05537	0.06281	0.81634	14	47	47
0.44462	0.06281	0.18366	14	48	48
0.44462	0.06281	0.81634	14	49	49
0.05537	0.06281	0.18366	14	50	50
0.94463	0.93719	0.18366	14	51	51
0.55537	0.93719	0.81634	14	52	52
0.56699	0.71656	0.00000	14	53	53
0.93301	0.71656	0.00000	14	54	54
0.06699	0.28344	0.00000	14	55	55
0.43301	0.28344	0.00000	14	56	56
0.56726	0.78317	0.11800	14	57	57
0.93274	0.78317	0.88200	14	58	58
0.06726	0.21683	0.88200	14	59	59
0.43274	0.21683	0.11800	14	60	60
0.43274	0.21683	0.88200	14	61	61
0.06726	0.21683	0.11800	14	62	62
0.93274	0.78317	0.11800	14	63	63
0.56726	0.78317	0.88200	14	64	64
0.56200	0.93286	0.04673	14	65	65
0.93800	0.93286	0.95327	14	66	66
0.06200	0.06714	0.95327	14	67	67
0.43800	0.06714	0.04673	14	68	68
0.43800	0.06714	0.95327	14	69	69
0.06200	0.06714	0.04673	14	70	70
0.93800	0.93286	0.04673	14	71	71
0.56200	0.93286	0.95327	14	72	72
0.56201	0.56710	0.07162	14	73	73
0.93799	0.56710	0.92838	14	74	74
0.06201	0.43290	0.92838	14	75	75
0.43799	0.43290	0.07162	14	76	76
0.43799	0.43290	0.92838	14	77	77
0.06201	0.43290	0.07162	14	78	78
0.93799	0.56710	0.07162	14	79	79
0.56201	0.56710	0.92838	14	80	80
0.55344	0.18209	0.07366	14	81	81
0.94656	0.18209	0.92634	14	82	82

0.05344	0.81791	0.92634	14	83	83
0.44656	0.81791	0.07366	14	84	84
0.44656	0.81791	0.92634	14	85	85
0.05344	0.81791	0.07366	14	86	86
0.94656	0.18209	0.07366	14	87	87
0.55344	0.18209	0.92634	14	88	88
0.55322	0.31790	0.04458	14	89	89
0.94678	0.31790	0.95542	14	90	90
0.05322	0.68210	0.95542	14	91	91
0.44678	0.68210	0.04458	14	92	92
0.44678	0.68210	0.95542	14	93	93
0.05322	0.68210	0.04458	14	94	94
0.94678	0.31790	0.04458	14	95	95
0.55322	0.31790	0.95542	14	96	96
0.55621	0.18155	0.16191	14	97	97
0.94379	0.18155	0.83809	14	98	98
0.05621	0.81845	0.83809	14	99	99
0.44379	0.81845	0.16191	14	100	100
0.44379	0.81845	0.83809	14	101	101
0.05621	0.81845	0.16191	14	102	102
0.94379	0.18155	0.16191	14	103	103
0.55621	0.18155	0.83809	14	104	104
0.25000	0.88108	0.14556	14	105	105
0.25000	0.88108	0.85444	14	106	106
0.75000	0.11892	0.85444	14	107	107
0.75000	0.11892	0.14556	14	108	108
0.25000	0.12585	0.11829	14	109	109
0.25000	0.12585	0.88170	14	110	110
0.75000	0.87415	0.88170	14	111	111
0.75000	0.87415	0.11829	14	112	112
0.25000	0.87951	0.09067	14	113	113
0.25000	0.87951	0.90933	14	114	114
0.75000	0.12049	0.90933	14	115	115
0.75000	0.12049	0.09067	14	116	116
0.25000	0.03268	0.07463	14	117	117
0.25000	0.03268	0.92537	14	118	118
0.75000	0.96732	0.92537	14	119	119
0.75000	0.96732	0.07463	14	120	120
0.25000	0.46758	0.04376	14	121	121
0.25000	0.46758	0.95624	14	122	122
0.75000	0.53243	0.95624	14	123	123
0.75000	0.53243	0.04376	14	124	124
0.25000	0.62067	0.02753	14	125	125
0.25000	0.62067	0.97247	14	126	126
0.75000	0.37933	0.97247	14	127	127
0.75000	0.37933	0.02753	14	128	128
0.25000	0.37468	0.00000	14	129	129
0.75000	0.62532	0.00000	14	130	130

S9.4 Ge-Clathrate/InN

S9.4.1 Thinner Ge Clathrate Film on InN (initial configuration)

See Figure S6.2.

10.89643	0.00000	-0.00000			
-5.44821	9.43658	0.00000			
0.00000	0.00000	26.29850			
95 atoms					
0.26262	0.13131	0.17022	32	1	1
0.86869	0.13131	0.17022	32	2	2
0.86869	0.73738	0.17022	32	3	3
0.66667	0.33333	0.21704	32	4	4
0.33333	0.66667	0.21710	32	5	5
0.41997	0.20999	0.24593	32	6	6
0.79002	0.20999	0.24593	32	7	7
0.79002	0.58003	0.24593	32	8	8
0.20999	0.41997	0.24594	32	9	9
0.20999	0.79002	0.24594	32	10	10
0.58003	0.79002	0.24594	32	11	11
0.39163	0.99998	0.28812	32	12	12
0.39163	0.39165	0.28812	32	13	13
0.60835	0.99998	0.28812	32	14	14
0.60835	0.60837	0.28812	32	15	15
0.00002	0.39165	0.28812	32	16	16
0.00002	0.60837	0.28812	32	17	17
0.00052	0.38429	0.04618	32	18	18
0.00052	0.61623	0.04618	32	19	19
0.38377	0.38429	0.04618	32	20	20
0.38377	0.99948	0.04618	32	21	21
0.61571	0.61623	0.04618	32	22	22
0.61571	0.99948	0.04618	32	23	23
0.41845	0.20923	0.09415	32	24	24
0.79077	0.20923	0.09415	32	25	25
0.79077	0.58155	0.09415	32	26	26
0.20914	0.41829	0.09469	32	27	27
0.20914	0.79086	0.09469	32	28	28
0.58171	0.79086	0.09469	32	29	29
0.66667	0.33333	0.12381	32	30	30
0.33333	0.66667	0.12389	32	31	31
0.13090	0.26180	0.17048	32	32	32
0.13090	0.86910	0.17048	32	33	33
0.73820	0.86910	0.17048	32	34	34
-0.77000	0.00000	0.35200	32	35	35
-0.76077	0.23947	0.35200	32	36	36
-0.23989	0.76044	0.35200	32	37	37
-0.23989	0.00000	0.35200	32	38	38

-0.03003	0.76052	0.35200	32	39	39
-0.03003	0.23956	0.35200	32	40	40
0.00000	0.00000	0.30200	32	41	41
0.66667	0.33333	0.73784	49	42	42
0.33333	0.66667	0.73561	49	43	43
0.00000	0.00000	0.73969	49	44	44
0.00385	0.33274	0.72373	49	45	45
0.00385	0.67111	0.72373	49	46	46
0.32889	0.33274	0.72373	49	47	47
0.32889	0.99615	0.72373	49	48	48
0.66726	0.67111	0.72373	49	49	49
0.66726	0.99615	0.72373	49	50	50
0.43857	0.21928	0.83677	49	51	51
0.78072	0.21928	0.83677	49	52	52
0.78072	0.56143	0.83677	49	53	53
0.11075	0.22151	0.84237	49	54	54
0.11075	0.88925	0.84237	49	55	55
0.77850	0.88925	0.84237	49	56	56
0.11170	0.55585	0.83822	49	57	57
0.44415	0.55585	0.83822	49	58	58
0.44415	0.88830	0.83822	49	59	59
0.56097	0.12193	0.94440	49	60	60
0.56097	0.43903	0.94440	49	61	61
0.87807	0.43903	0.94440	49	62	62
0.22710	0.45421	0.95022	49	63	63
0.22710	0.77290	0.95022	49	64	64
0.54580	0.77290	0.95022	49	65	65
0.21562	0.10781	0.95497	49	66	66
0.89219	0.10781	0.95497	49	67	67
0.89219	0.78438	0.95497	49	68	68
0.11198	0.22396	0.75643	7	69	69
0.11198	0.88802	0.75643	7	70	70
0.77604	0.88802	0.75643	7	71	71
0.43990	0.21995	0.75028	7	72	72
0.78005	0.21995	0.75028	7	73	73
0.78005	0.56010	0.75028	7	74	74
0.10927	0.55463	0.75192	7	75	75
0.44537	0.55463	0.75192	7	76	76
0.44537	0.89073	0.75192	7	77	77
0.55592	0.11184	0.86040	7	78	78
0.55592	0.44408	0.86040	7	79	79
0.88816	0.44408	0.86040	7	80	80
0.22427	0.11213	0.86930	7	81	81
0.88787	0.11213	0.86930	7	82	82
0.88787	0.77573	0.86930	7	83	83
0.22254	0.44508	0.86554	7	84	84
0.22254	0.77746	0.86554	7	85	85
0.55492	0.77746	0.86554	7	86	86
0.33884	0.00024	0.97522	7	87	87

0.33884	0.33860	0.97522	7	88	88
0.66140	0.00024	0.97522	7	89	89
0.66140	0.66116	0.97522	7	90	90
0.99976	0.33860	0.97522	7	91	91
0.99976	0.66116	0.97522	7	92	92
0.00000	0.00000	0.98093	7	93	93
0.66667	0.33333	0.97516	7	94	94
0.33333	0.66667	0.98001	7	95	95

S9.4.2 Thicker Ge Clathrate Film on InN (initial configuration)

See Figure S6.6.

10.89643	0.00000	-0.00000			
-5.44821	9.43658	0.00000			
0.00000	0.00000	50.00000			
129 atoms					
1.00700	1.00700	0.36991	32	1	1
0.34644	0.06187	0.16999	32	2	2
-0.04787	0.29157	0.16999	32	3	3
-0.27757	-0.33244	0.16999	32	4	4
-0.27757	0.06187	0.16999	32	5	5
0.34644	0.29157	0.16999	32	6	6
-0.04787	-0.33244	0.16999	32	7	7
-0.04176	0.28546	0.03126	32	8	8
0.33423	0.05576	0.03126	32	9	9
-0.27146	-0.32023	0.03126	32	10	10
0.33423	0.28546	0.03126	32	11	11
-0.27146	0.05576	0.03126	32	12	12
-0.04176	-0.32023	0.03126	32	13	13
-0.37510	-0.38120	0.21851	32	14	14
0.00089	0.38910	0.21851	32	15	15
0.39520	0.01311	0.21851	32	16	16
0.00089	-0.38120	0.21851	32	17	17
0.39520	0.38910	0.21851	32	18	18
-0.37510	0.01311	0.21851	32	19	19
-0.45167	0.46567	0.05657	32	20	20
-0.45167	0.08966	0.05657	32	21	21
-0.07566	0.46567	0.05657	32	22	22
0.21500	-0.20100	0.24382	32	23	23
0.21500	0.42299	0.24382	32	24	24
-0.40899	-0.20100	0.24382	32	25	25
-0.24367	-0.11834	0.14468	32	26	26
0.13234	0.25767	0.14468	32	27	27
0.13234	-0.11834	0.14468	32	28	28
0.00700	0.00700	0.07722	32	29	29
-0.32633	0.34033	0.26447	32	30	30

-0.32633	0.34033	0.12403	32	31	31
-0.44907	0.46307	0.14127	32	32	32
-0.44907	0.09486	0.14127	32	33	33
-0.08086	0.46307	0.14127	32	34	34
-0.23847	-0.11574	0.05998	32	35	35
0.12974	0.25247	0.05998	32	36	36
0.12974	-0.11574	0.05998	32	37	37
0.42819	0.21760	0.24723	32	38	38
-0.20360	-0.41419	0.24723	32	39	39
-0.20360	0.21760	0.24723	32	40	40
0.00700	0.00700	0.12893	32	41	41
-0.32633	0.34033	0.07232	32	42	42
0.34033	-0.32633	0.25957	32	43	43
0.47177	-0.45777	0.09958	32	44	44
0.47177	-0.06346	0.09958	32	45	45
0.07746	-0.45777	0.09958	32	46	46
0.13844	-0.12444	0.28683	32	47	47
0.13844	0.26987	0.28683	32	48	48
-0.25587	-0.12444	0.28683	32	49	49
-0.39679	-0.19490	0.10167	32	50	50
0.20890	0.41079	0.10167	32	51	51
0.20890	-0.19490	0.10167	32	52	52
0.01311	0.39520	0.35723	32	53	53
-0.38120	-0.37510	0.35723	32	54	54
0.38910	0.00089	0.35723	32	55	55
0.38910	0.39520	0.35723	32	56	56
0.01311	-0.37510	0.35723	32	57	57
-0.38120	0.00089	0.35723	32	58	58
0.42299	0.21500	0.33193	32	59	59
-0.20100	-0.40899	0.33193	32	60	60
-0.20100	0.21500	0.33193	32	61	61
0.34033	-0.32633	0.31128	32	62	62
0.21760	-0.20360	0.32852	32	63	63
0.21760	0.42819	0.32852	32	64	64
-0.41419	-0.20360	0.32852	32	65	65
-0.32633	0.34033	0.31618	32	66	66
0.26987	0.13844	0.28892	32	67	67
-0.12444	-0.25587	0.28892	32	68	68
-0.12444	0.13844	0.28892	32	69	69
0.76744	1.76743	0.39949	32	70	70
0.76744	1.00700	0.39949	32	71	71
1.00700	1.76743	0.39949	32	72	72
1.00700	1.24656	0.39949	32	73	73
0.24656	1.00700	0.39949	32	74	74
0.24656	1.24656	0.39949	32	75	75
0.66667	0.33333	-0.13789	49	76	76
0.33333	0.66667	-0.13906	49	77	77
0.00000	0.00000	-0.13692	49	78	78
0.00385	0.33274	-0.14531	49	79	79
0.00385	0.67111	-0.14531	49	80	80

0.32889	0.33274	-0.14531	49	81	81
0.32889	0.99615	-0.14531	49	82	82
0.66726	0.67111	-0.14531	49	83	83
0.66726	0.99615	-0.14531	49	84	84
0.43857	0.21928	-0.08586	49	85	85
0.78072	0.21928	-0.08586	49	86	86
0.78072	0.56143	-0.08586	49	87	87
0.11075	0.22151	-0.08291	49	88	88
0.11075	0.88925	-0.08291	49	89	89
0.77850	0.88925	-0.08291	49	90	90
0.11170	0.55585	-0.08509	49	91	91
0.44415	0.55585	-0.08509	49	92	92
0.44415	0.88830	-0.08509	49	93	93
0.56097	0.12193	-0.02925	49	94	94
0.56097	0.43903	-0.02925	49	95	95
0.87807	0.43903	-0.02925	49	96	96
0.22710	0.45421	-0.02618	49	97	97
0.22710	0.77290	-0.02618	49	98	98
0.54580	0.77290	-0.02618	49	99	99
0.21562	0.10781	-0.02368	49	100	100
0.89219	0.10781	-0.02368	49	101	101
0.89219	0.78438	-0.02368	49	102	102
0.11198	0.22396	-0.12811	7	103	103
0.11198	0.88802	-0.12811	7	104	104
0.77604	0.88802	-0.12811	7	105	105
0.43990	0.21995	-0.13134	7	106	106
0.78005	0.21995	-0.13134	7	107	107
0.78005	0.56010	-0.13134	7	108	108
0.10927	0.55463	-0.13049	7	109	109
0.44537	0.55463	-0.13049	7	110	110
0.44537	0.89073	-0.13049	7	111	111
0.55592	0.11184	-0.07343	7	112	112
0.55592	0.44408	-0.07343	7	113	113
0.88816	0.44408	-0.07343	7	114	114
0.22427	0.11213	-0.06875	7	115	115
0.88787	0.11213	-0.06875	7	116	116
0.88787	0.77573	-0.06875	7	117	117
0.22254	0.44508	-0.07072	7	118	118
0.22254	0.77746	-0.07072	7	119	119
0.55492	0.77746	-0.07072	7	120	120
0.33884	0.00024	-0.01303	7	121	121
0.33884	0.33860	-0.01303	7	122	122
0.66140	0.00024	-0.01303	7	123	123
0.66140	0.66116	-0.01303	7	124	124
0.99976	0.33860	-0.01303	7	125	125
0.99976	0.66116	-0.01303	7	126	126
0.00000	0.00000	-0.01003	7	127	127
0.66667	0.33333	-0.01307	7	128	128
0.33333	0.66667	-0.01051	7	129	129

S10. Tabulated $E(\rho)$ Dependencies

S10.1 $E(\rho)$ of Sn

ρ [at./Å^2]	ρ [ML]	E_{KS} [eV/at.]	$E - E_{\mathrm{bulk}}$ [meV/at.]	E_{g} [eV]	sample designation
0.1422	1.356	-3.6043	265	0.038	db-monolayer (oP10)
0.1741	1.660	-3.6159	253	0.000	db-monolayer (hP11)
0.1425	1.358	-3.6268	242	0.065	Sn9-web (40 atoms)
0.1749	1.667	-3.6530	216	0.000	Sn9-web (100 atoms)
0.2224	2.120	-3.6707	198	0.000	triangles (bilayer)
0.4449	4.241	-3.7092	160	0.000	triangles (2×bilayer)
0.2448	2.334	-3.7103	159	0.000	squares (bilayer)
0.4850	4.623	-3.7384	130	0.000	squares (2×bilayer)
0.7115	6.783	-3.7499	119	0.000	squares (3×bilayer)
0.3428	3.268	-3.7268	142	0.000	Sn.equi-II-3
0.5501	5.244	-3.7731	96	0.250	Sn.equi-II-5
0.7981	7.608	-3.7934	75	0.263	Sn.equi-II-7.5
1.0470	9.981	-3.8041	65	0.266	Sn.equi-II-10
0.2629	2.506	-3.6568	212	0.000	$(\sqrt{3} \times \sqrt{3})$-dia (bilayer)
0.2578	2.458	-3.6219	247	0.000	(2×2)-dia (bilayer)
0.3578	3.411	-3.6906	178	0.000	(2×2)-dia (trilayer)
0.4618	4.402	-3.7257	143	0.000	(2×2)-dia (fourlayer)
0.5663	5.398	-3.7512	118	0.000	(2×2)-dia (fivelayer)
0.6705	6.392	-3.7674	101	0.000	(2×2)-dia (sixlayer)
0.7754	7.392	-3.7810	88	0.000	(2×2)-dia (sevenlayer)
0.8803	8.392	-3.7909	78	0.000	(2×2)-dia (eightlayer)
0.9854	9.394	-3.7986	70	0.000	(2×2)-dia (ninelayer)

Table S10.1: *Tabulated content of Figure 6 (main text) for Sn thin films. "KS" denotes total Kohn-Sham energy as a direct output of VASP (without dispersion vdW correction). For unit conversion: thickness of* 1ML *of (111)-diamond cF8 Sn is* $\rho_0 = 0.10490\,\mathrm{at./Å^2}$ *and the respective bulk Kohn-Sham per-atom energy* $E_{\mathrm{bulk}} = -3.8688\,\mathrm{eV/at.}$ E_{g} *stands for the width of electronic band gap.*

S10.2 $E(\rho)$ of Ge

ρ [at./Å^2]	ρ [ML]	E_{KS} [eV/at.]	$E - E_{bulk}$ [meV/at.]	E_g [eV]	sample designation
0.1884	1.359	-4.2083	308	0.100	db-monolayer (oP10)
0.2367	1.707	-4.1636	352	0.000	GS-bilayer
0.3534	2.549	-4.2648	251	0.256	Ge.iso-II-2.5
0.4037	2.911	-4.2941	222	0.400	Ge.equi-II-3
0.4781	3.448	-4.3328	183	0.428	Ge.equi-II-3.5
0.5461	3.938	-4.3404	176	0.217	Ge.iso-II-4
0.8042	5.800	-4.3957	120	0.517	Ge.equi-II-6
0.3455	2.492	-4.2535	262	0.000	$(\sqrt{3} \times \sqrt{3})$-dia (bilayer)
0.3331	2.402	-4.2252	291	0.133	(2×2)-dia (bilayer)
0.4683	3.377	-4.2950	221	0.000	(2×2)-dia (trilayer)
0.6059	4.370	-4.3404	176	0.000	(2×2)-dia (fourlayer)
0.7440	5.366	-4.3736	142	0.000	(2×2)-dia (fivelayer)
0.8822	6.362	-4.3948	121	0.000	(2×2)-dia (sixlayer)
1.0208	7.362	-4.4118	104	0.022	(2×2)-dia (sevenlayer)
1.1585	8.355	-4.4245	91	0.057	(2×2)-dia (eightlayer)
1.2982	9.362	-4.4343	82	0.108	(2×2)-dia (ninelayer)

Table S10.2.1: *Tabulated content of Figure 6 (main text) for Ge thin films. "KS" denotes total Kohn-Sham energy as a direct output of VASP (without dispersion vdW correction). For unit conversion: thickness of* 1ML *of (111)-diamond cF8 Ge is* $\rho_0 = 0.13866$at./Å^2 *and the respective bulk Kohn-Sham per-atom energy* $E_{bulk} = -4.5159$ eV/at. E_g *stands for the width of electronic band gap.*

ρ [at./Å^2]	ρ [ML]	E_{KS} [eV/at.]	$E - E_{bulk}$ [meV/at.]	E_g [eV]	sample designation
0.1924	1.361	-4.3810	389	0.000	db-monolayer (oP10)
0.3591	2.540	-4.4461	323	0.000	Ge.iso-II-2.5
0.5612	3.970	-4.5343	235	0.255	Ge.iso-II-4
0.7908	5.595	-4.5855	184	0.435	Ge.iso-II-5.5
0.4107	2.905	-4.4844	285	0.455	Ge.equi-II-3
0.4912	3.475	-4.5313	238	0.490	Ge.equi-II-3.5
0.8137	5.756	-4.5952	174	0.450	Ge.equi-II-6
0.3510	2.483	-4.4444	325	0.000	$(\sqrt{3} \times \sqrt{3})$-dia (bilayer)
0.4771	3.374	-4.5069	263	0.000	(2×2)-dia (trilayer)
0.6320	4.471	-4.5609	209	0.000	$(\sqrt{3} \times \sqrt{3})$-dia (fourlayer)
0.7712	5.456	-4.5959	174	0.000	$(\sqrt{3} \times \sqrt{3})$-dia (fivelayer)
1.0492	7.422	-4.6433	126	0.000	$(\sqrt{3} \times \sqrt{3})$-dia (sevenlayer)
0.4276	3.025	-4.4632	307	0.000	(3×3)-DAS (trilayer)
0.5650	3.997	-4.5296	240	0.000	(3×3)-DAS (fourlayer)

Table S10.2.2: *Tabulated content of Figure S7.1 (SM) for Ge thin films. "KS" denotes total Kohn-Sham energy as a direct output of VASP,* with *dispersion vdW correction (PBE-*

D3, `IVDW=12`). For unit conversion: thickness of 1 ML *of (111)-diamond cF8 Ge is* $\rho_0 = 0.141357\,\text{at.}/\text{Å}^2$ *and the respective bulk Kohn-Sham per-atom energy* $E_{\text{bulk}} = -4.7696\,\text{eV/at.}$ E_{g} *stands for the width of electronic band gap.*

S10.3 $E(\rho)$ of Si

ρ [at./Å^2]	ρ [ML]	E_{KS} [eV/at.]	$E - E_{\text{bulk}}$ [meV/at.]	E_{g} [eV]	sample designation
0.2110	1.364	-4.9906	430	0.650	db-monolayer (oP10)
0.2709	1.751	-4.9566	464	0.000	GS-bilayer
0.3851	2.489	-5.0987	322	0.467	Si.iso-II-2.5
0.5032	3.253	-5.1399	280	0.950	Si.equi-II-3
0.6056	3.915	-5.1885	232	0.837	Si.iso-II-4
0.8272	5.347	-5.2338	186	0.762	Si.iso-II-5
0.3866	2.499	-5.0643	356	0.138	$(\sqrt{3} \times \sqrt{3})$-dia (bilayer)
0.3690	2.385	-5.0080	412	0.000	(2×2)-dia (bilayer)
0.5263	3.402	-5.1245	296	0.450	(2×2)-dia (trilayer)
0.6788	4.388	-5.1834	237	0.300	(2×2)-dia (fourlayer)
0.8339	5.391	-5.2279	192	0.465	(2×2)-dia (fivelayer)
0.9874	6.383	-5.2561	164	0.436	(2×2)-dia (sixlayer)
1.1423	7.384	-5.2792	141	0.450	(2×2)-dia (sevenlayer)
1.2969	8.384	-5.2961	124	0.473	(2×2)-dia (eightlayer)
1.4515	9.383	-5.3094	111	0.480	(2×2)-dia (ninelayer)

Table S10.3.1: *Tabulated content of Figure 6 (main text) for Si thin films. "KS" denotes total Kohn-Sham energy as a direct output of VASP (without dispersion vdW correction). For unit conversion: thickness of* 1 ML *of (111)-diamond cF8 Si is* $\rho_0 = 0.15469\,\text{at.}/\text{Å}^2$ *and the respective bulk Kohn-Sham per-atom energy* $E_{\text{bulk}} = -5.4202\,\text{eV/at.}$ E_{g} *stands for the width of electronic band gap.*

ρ [at./Å^2]	ρ [ML]	E_{KS} [eV/at.]	$E - E_{\text{bulk}}$ [meV/at.]	E_{g} [eV]	sample designation
0.2127	1.351	-5.1751	550	0.508	db-monolayer (oP10)
0.3903	2.479	-5.3273	398	0.371	Si.iso-II-2.5
0.6131	3.894	-5.4256	300	0.787	Si.iso-II-4
0.8376	5.320	-5.4762	249	0.731	Si.iso-II-5.5
0.5105	3.242	-5.3773	348	0.950	Si.equi-II-3
0.5381	3.417	-5.3957	329	0.847	Si.equi-II-3.5
0.3919	2.488	-5.3044	421	0.000	$(\sqrt{3} \times \sqrt{3})$-dia (bilayer)
0.5356	3.402	-5.3874	338	0.420	(2×2)-dia (trilayer)
0.8462	5.374	-5.5051	220	0.334	$c(2 \times 4)$-dia (fivelayer)
0.4755	3.020	-5.3460	379	0.000	(3×3)-DAS (trilayer)
0.6305	4.004	-5.4274	298	0.000	(3×3)-DAS (fourlayer)
0.4435	2.817	-5.2692	456	0.034	a-Si (trilayer)
0.6143	3.901	-5.3652	360	0.070	a-Si (fourlayer, cF8 nuclei)

Table S10.3.2: *Tabulated content of Figure S7.1 (SM) for Si thin films. "KS" denotes total Kohn-Sham energy as a direct output of VASP,* with *dispersion vdW correction (PBE-D3,* `IVDW=12`*). For unit conversion: thickness of* 1 ML *of (111)-diamond cF8 Si is* $\rho_0 = 0.157457$ at./Å^2 *and the respective bulk Kohn-Sham per-atom energy* $E_{\mathrm{bulk}} = -5.7251$ eV/at. E_{g} *stands for the width of electronic band gap.*