Electronic Supplementary Information

A new calculation strategy to analyze the vibrational free energy of a slab and calculate the vibrational contribution of the surface free energy

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CRYSTAL Computational details (LiF slab)

The multielectronic wave function is constructed as an antisymmetrized product (Slater determinant) of monoelectronic crystalline orbitals (CO) which are linear combinations of local functions (to be indicated as AO's) centered on each atom of the crystal. In turn, AO's (basis set) are linear combinations of Gaussian-type functions (GTF, the product of a Gaussian times a real solid spherical harmonic to give s-, p-, and d-type AO's).

Li is described with a 6-11G* basis.[1] It consists of six contracted GTF's for the description of the core s shell, and two uncontracted sp and one d functions for the valence shell. For F, the basis sets used is 7-311G*[2] consisting of seven contracted GTF's for the description of the core s shell, and a contraction of three and two uncontracted sp's, and one d function for the valence shell. All of the exponents of the valence sp and d GTF's have been variationally optimized.

The calculations were performed at the Hartree-Fock level. The five parameters (ITOL1, ITOL2, ITOL3, ITOL4, and ITOL5) controlling the accuracy of the calculation of Coulomb and exchange integrals[3] were set to 10^{-8} (ITOL1 to ITOL4) and 10^{-16} (ITOL5). The diagonalization of the Fock matrix was performed at 10 **k** points in the reciprocal space (Monkhrost net[4]) by setting the shrinking factor IS[3] to 8. For both geometry and frequency calculations, the SCF convergence threshold on total energy (TOLDEE in CRYSTAL06) has been set to 10^{-10} bohr. Geometry optimization is achieved when each of the components of the gradient and of the displacement (TOLDEG, TOLDEX parameters in CRYSTAL06) are smaller than 4×10^{-5} hartree bohr^{-1} and 10^{-5} bohr, respectively.

CRYSTAL06[3,5] computes numerically the second derivatives of the energy using analytical first derivatives. The calculation is done by displacing the irreducible atoms only. The full mass-weighted Hessian matrix, in Cartesian coordinates, is then generated and diagonalized to obtain eigenvalues and normal modes. The frequencies must be computed when the crystalline structure is at a minimum on the potential energy surface. Therefore, harmonic frequency calculations have been performed on the optimized (100) slab.

References

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Table S1. Vibrational energy (E_j^{vib}), entropy (S_j^{vib}) and free energy (F_j^{vib}) at T = 298.15 K of Li and F atoms forming the (100) slab of LiF. The slab is composed by 28 layers and 56 atoms (a LiF molecule per layer) related by an inversion center. Here, only the symmetrically independent layers (*l* = 1, …, 14, where *l* = 1 is the surface layer) and atoms (*j* = 1, …, 28; where the atoms 1 and 2 are in the surface layer *l* =1) are reported.

atom number	atom type	layer	E_j^{vib} (J/mol)	S_j^{vib} (J/mol/K)	F_j^{vib} (J/mol)
1	LI	1	11910.6970	31.6228	2482.3593
2	F	1	5197.1686	23.4219	-1786.0735
3	LI	2	11864.9940	26.1043	4081.9833
4	F	2	5644.7988	20.0681	-338.5047
5	LI	3	12029.0570	25.8011	4336.4458
6	F	3	5628.3549	19.3197	-131.8203
7	LI	4	12012.8030	25.3864	4443.8563
8	F	4	5644.6972	18.9715	-11.6604
9	LI	5	12012.6180	25.2069	4497.1823
10	F	5	5643.4786	18.7913	40.8605
11	LI	6	12014.6200	25.0776	4537.7366
12	F	6	5646.0078	18.6698	79.5980
13	LI	7	12015.8110	25.0034	4561.0391
14	F	7	5644.9418	18.5936	101.2489
15	LI	8	12015.2880	24.9511	4576.1309
16	F	8	5647.4423	18.5493	116.9549
17	LI	9	12020.8020	24.9251	4589.3861
18	F	9	5645.6095	18.5095	126.9994
19	LI	10	12015.8650	24.8950	4593.4249
20	F	10	5650.4977	18.4876	138.4077
21	LI	11	12018.4850	24.8782	4601.0399
22	F	11	5650.5198	18.4823	140.0150
23	LI	12	12019.0570	24.8768	4602.0407
24	F	12	5649.3912	18.4599	145.5855
25	LI	13	12017.8770	24.8610	4605.5694
26	F	13	5653.2232	18.4593	149.5829
27	LI	14	12020.6040	24.8374	4615.3215
28	F	14	5652.3528	18.4423	153.7909
		Σ	246587.0630	625.6534	60048.5009

Table S2. Vibrational energy (E_l^{vib}), entropy (S_l^{vib}) and free energy (F_l^{vib}) at T = 298.15 K of the layers forming the (100) slab of LiF. The slab is composed by 28 layers (a LiF molecule per layer) related by an inversion center. Here, only the symmetrically independent layers (*l* = 1, …, 14, where *l* = 1 is the surface layer) are reported. The percentage contribution of each layer to the vibrational energy (E=100× E_l^{vib}/Σ), entropy (S=100× S_l^{vib}/Σ) and free energy (F=100× F_l^{vib}/Σ) of the slab is also reported.

layer	E_l^{vib} (J/mol)	S_l^{vib} (J/mol/K)	F_l^{vib} (J/mol)	E (%)	S (%)	F (%)
1	17107.8660	55.0447	696.2858	6.9379	8.7980	1.1595
2	17509.7920	46.1724	3743.4786	7.1009	7.3799	6.2341
3	17657.4120	45.1209	4204.6255	7.1607	7.2118	7.0020
4	17657.5000	44.3579	4432.1959	7.1608	7.0899	7.3810
5	17656.0970	43.9982	4538.0428	7.1602	7.0324	7.5573
6	17660.6280	43.7474	4617.3346	7.1620	6.9923	7.6893
7	17660.7530	43.5971	4662.2880	7.1621	6.9682	7.7642
8	17662.7310	43.5004	4693.0858	7.1629	6.9528	7.8155
9	17666.4120	43.4346	4716.3855	7.1644	6.9423	7.8543
10	17666.3620	43.3826	4731.8326	7.1644	6.9340	7.8800
11	17669.0050	43.3606	4741.0549	7.1654	6.9304	7.8954
12	17668.4490	43.3367	4747.6263	7.1652	6.9266	7.9063
13	17671.1000	43.3203	4755.1523	7.1663	6.9240	7.9189
14	17672.9560	43.2797	4769.1123	7.1670	6.9175	7.9421
Σ	246587.0630	625,6534	60048,5009	100,0000	100,0000	100,0000

Table S3. Vibrational energy (E_j^{vib}), entropy (S_j^{vib}) and free energy (F_j^{vib}) at T = 300 K of Ca, C and O atoms forming the (10.4) slab of calcite. The slab is composed by 10 layers (*l* = 1, …, 10, where *l* = 1 is the surface layer) and 300 atoms (*j* = 1, …, 300; where the atoms 1-30 are in the surface layer *l* =1; six CaCO3 molecules per layer) both in the region 1 and 2. Here, only the atoms of the region 1, which are allowed to relax according to the GULP strategy, are reported.

atom number	atom type	layer	E_j^{vib} (J/mol)	S_j^{vib} (J/mol/K)	F_j^{vib} (J/mol)
1	O	1	11729.5690	24.1401	4487.5437
2	O	1	11729.5690	24.1401	4487.5394
3	O	1	11728.0230	24.0732	4506.0662
4	O	1	11728.0240	24.0732	4506.0734
5	O	1	11729.5690	24.1401	4487.5517
6	O	1	11728.0230	24.0732	4506.0594
7	Ca	1	8316.7364	30.0713	-704.6557
8	O	1	11714.5370	19.8868	5748.4957
9	C	1	18743.1950	8.7478	16118.8660
10	O	1	11714.5350	19.8868	5748.4950
11	C	1	18743.1980	8.7478	16118.8680
12	O	1	11712.1630	19.8760	5749.3630
13	C	1	18743.1460	8.7417	16120.6260
14	Ca	1	8316.7367	30.0713	-704.6546
15	Ca	1	8313.7962	30.1190	-721.8980
16	Ca	1	8313.7964	30.1190	-721.8992
17	O	1	11712.1610	19.8760	5749.3568
18	C	1	18743.1440	8.7417	16120.6230
19	O	1	11714.5360	19.8868	5748.4966
20	C	1	18743.1950	8.7478	16118.8640
21	O	1	11712.1620	19.8760	5749.3588
22	C	1	18743.1460	8.7417	16120.6260
23	Ca	1	8313.7956	30.1190	-721.8975
24	Ca	1	8316.7364	30.0713	-704.6554
25	O	1	11722.6760	20.8366	5471.6828
26	O	1	11719.1520	20.7890	5482.4547
27	O	1	11719.1530	20.7890	5482.4582
28	O	1	11722.6740	20.8367	5471.6732
29	O	1	11719.1520	20.7890	5482.4466
30	O	1	11722.6740	20.8366	5471.6807
31	O	2	11815.5060	19.6599	5917.5211
32	O	2	11815.5070	19.6599	5917.5231
33	O	2	11815.7610	19.6604	5917.6437
34	O	2	11815.7620	19.6604	5917.6409
35	O	2	11815.5080	19.6599	5917.5257
36	O	2	11815.7610	19.6604	5917.6390
37	Ca	2	8374.9968	27.5134	120.9858
38	Ca	2	8374.9951	27.5134	120.9883
39	O	2	11808.8970	19.2095	6046.0333

40	C	2	18704.9280	8.2761	16222.1000
41	O	2	11808.8960	19.2095	6046.0330
42	C	2	18704.9270	8.2761	16222.0990
43	Ca	2	8373.1366	27.5233	116.1568
44	O	2	11808.1360	19.2151	6043.6082
45	C	2	18704.5610	8.2768	16221.5310
46	Ca	2	8373.1381	27.5233	116.1547
47	O	2	11808.1370	19.2151	6043.6038
48	C	2	18704.5640	8.2768	16221.5330
49	O	2	11808.1350	19.2151	6043.6028
50	C	2	18704.5640	8.2768	16221.5330
51	Ca	2	8373.1362	27.5233	116.1561
52	Ca	2	8374.9981	27.5134	120.9867
53	O	2	11808.8960	19.2095	6046.0335
54	C	2	18704.9260	8.2761	16222.0990
55	O	2	11800.9800	19.2052	6039.4297
56	O	2	11801.5390	19.1966	6042.5620
57	O	2	11800.9770	19.2052	6039.4258
58	O	2	11801.5370	19.1966	6042.5607
59	O	2	11801.5390	19.1966	6042.5630
60	O	2	11800.9760	19.2052	6039.4297
61	O	3	11762.2210	19.2682	5981.7646
62	O	3	11762.2220	19.2682	5981.7628
63	O	3	11762.4730	19.2738	5980.3464
64	O	3	11762.4720	19.2738	5980.3446
65	O	3	11762.2210	19.2682	5981.7654
66	O	3	11762.4750	19.2738	5980.3454
67	Ca	3	8370.8353	27.2824	186.1259
68	Ca	3	8370.8363	27.2824	186.1272
69	O	3	11781.5580	19.0187	6075.9562
70	C	3	18608.9530	8.2755	16126.2970
71	O	3	11781.5580	19.0187	6075.9566
72	C	3	18608.9510	8.2755	16126.2950
73	Ca	3	8370.3900	27.2856	184.7113
74	O	3	11781.3170	19.0212	6074.9673
75	C	3	18609.5160	8.2763	16126.6260
76	O	3	11781.3170	19.0212	6074.9675
77	C	3	18609.5150	8.2763	16126.6250
78	Ca	3	8370.3906	27.2856	184.7112
79	Ca	3	8370.3907	27.2856	184.7102
80	Ca	3	8370.8345	27.2824	186.1273
81	O	3	11781.5550	19.0187	6075.9562
82	C	3	18608.9530	8.2755	16126.2980
83	O	3	11781.3160	19.0212	6074.9667
84	C	3	18609.5170	8.2763	16126.6260
85	O	3	11761.7640	19.2253	5994.1809
86	O	3	11761.7500	19.2282	5993.3018

87	O	3	11761.7510	19.2282	5993.3043
88	O	3	11761.7630	19.2253	5994.1827
89	O	3	11761.7500	19.2282	5993.2993
90	O	3	11761.7640	19.2253	5994.1822
91	O	4	11784.7430	19.1862	6028.8895
92	O	4	11784.7440	19.1862	6028.8868
93	O	4	11784.4010	19.1845	6029.0578
94	O	4	11784.4010	19.1845	6029.0603
95	O	4	11784.7450	19.1862	6028.8921
96	O	4	11784.4000	19.1845	6029.0550
97	Ca	4	8367.0534	27.2083	204.5574
98	O	4	11781.9370	19.0495	6067.0973
99	C	4	18601.5820	8.2858	16115.8350
100	O	4	11781.9370	19.0495	6067.0916
101	C	4	18601.5820	8.2858	16115.8340
102	Ca	4	8367.0542	27.2083	204.5576
103	Ca	4	8366.3276	27.2157	201.6067
104	O	4	11782.0800	19.0485	6067.5411
105	C	4	18601.3380	8.2864	16115.4080
106	O	4	11782.0830	19.0485	6067.5454
107	C	4	18601.3380	8.2864	16115.4080
108	Ca	4	8366.3268	27.2157	201.6055
109	Ca	4	8366.3272	27.2157	201.6050
110	Ca	4	8367.0545	27.2083	204.5571
111	O	4	11781.9360	19.0495	6067.0928
112	C	4	18601.5850	8.2858	16115.8370
113	O	4	11782.0830	19.0485	6067.5472
114	C	4	18601.3390	8.2864	16115.4080
115	O	4	11783.9510	19.1997	6024.0551
116	O	4	11783.6480	19.1945	6025.2835
117	O	4	11783.6480	19.1945	6025.2834
118	O	4	11783.9510	19.1997	6024.0555
119	O	4	11783.9510	19.1997	6024.0547
120	O	4	11783.6470	19.1945	6025.2840
121	O	5	11764.1990	19.2286	5995.6051
122	O	5	11764.0690	19.2312	5994.7236
123	O	5	11764.0690	19.2312	5994.7236
124	O	5	11764.0700	19.2311	5994.7248
125	O	5	11764.2020	19.2286	5995.6101
126	O	5	11764.2000	19.2287	5995.6033
127	Ca	5	8372.3355	27.1373	231.1517
128	Ca	5	8372.3356	27.1373	231.1535
129	O	5	11780.3220	18.9971	6081.1773
130	C	5	18577.7890	8.2902	16090.7370
131	O	5	11780.3670	18.9981	6080.9430
132	C	5	18577.9880	8.2905	16090.8420
133	Ca	5	8371.9902	27.1400	229.9858

134	Ca	5	8371.9900	27.1400	229.9853
135	Ca	5	8372.3359	27.1373	231.1524
136	O	5	11780.3680	18.9981	6080.9460
137	C	5	18577.9850	8.2905	16090.8410
138	O	5	11780.3230	18.9972	6081.1744
139	C	5	18577.7880	8.2902	16090.7360
140	O	5	11780.3670	18.9981	6080.9437
141	C	5	18577.9860	8.2905	16090.8410
142	Ca	5	8371.9905	27.1400	229.9873
143	O	5	11780.3210	18.9972	6081.1728
144	C	5	18577.7860	8.2902	16090.7350
145	O	5	11764.5050	19.2015	6004.0406
146	O	5	11764.6480	19.2031	6003.7116
147	O	5	11764.5060	19.2015	6004.0415
148	O	5	11764.6490	19.2031	6003.7168
149	O	5	11764.5060	19.2016	6004.0358
150	O	5	11764.6480	19.2031	6003.7092
151	O	6	11779.3030	19.1730	6027.4178
152	O	6	11779.3030	19.1729	6027.4197
153	O	6	11779.4040	19.1717	6027.8817
154	O	6	11779.4040	19.1717	6027.8852
155	O	6	11779.3030	19.1729	6027.4181
156	O	6	11779.4040	19.1718	6027.8780
157	Ca	6	8367.7390	27.1601	219.7237
158	Ca	6	8367.7390	27.1601	219.7233
159	O	6	11780.4340	19.0154	6075.8097
160	C	6	18579.8200	8.2951	16091.2910
161	O	6	11780.3740	19.0146	6075.9815
162	C	6	18579.8500	8.2950	16091.3520
163	Ca	6	8367.5957	27.1613	219.2097
164	Ca	6	8367.5951	27.1613	219.2086
165	Ca	6	8367.7388	27.1600	219.7240
166	O	6	11780.3750	19.0146	6075.9819
167	C	6	18579.8500	8.2950	16091.3520
168	O	6	11780.4320	19.0154	6075.8064
169	C	6	18579.8180	8.2951	16091.2880
170	O	6	11780.3760	19.0146	6075.9841
171	C	6	18579.8480	8.2950	16091.3510
172	Ca	6	8367.5954	27.1613	219.2093
173	O	6	11780.4330	19.0154	6075.8066
174	C	6	18579.8160	8.2951	16091.2860
175	O	6	11778.8400	19.1855	6023.2002
176	O	6	11778.9360	19.1848	6023.5112
177	O	6	11778.8390	19.1855	6023.2020
178	O	6	11778.9350	19.1848	6023.5072
179	O	6	11778.9370	19.1848	6023.5082
180	O	6	11778.8380	19.1855	6023.1948

181	O	7	11766.5640	19.2028	6005.7361
182	O	7	11766.3330	19.2032	6005.3748
183	O	7	11766.3330	19.2032	6005.3790
184	O	7	11766.5620	19.2028	6005.7325
185	O	7	11766.3340	19.2032	6005.3787
186	O	7	11766.5630	19.2028	6005.7304
187	Ca	7	8371.7330	27.1024	240.9982
188	Ca	7	8371.7330	27.1024	240.9983
189	O	7	11779.9030	18.9829	6085.0345
190	C	7	18568.6590	8.2931	16080.7340
191	O	7	11779.8420	18.9839	6084.6570
192	C	7	18568.4860	8.2933	16080.5070
193	Ca	7	8371.6518	27.1033	240.6630
194	Ca	7	8371.6512	27.1033	240.6623
195	Ca	7	8371.7330	27.1024	240.9990
196	O	7	11779.8430	18.9839	6084.6609
197	C	7	18568.4840	8.2933	16080.5070
198	O	7	11779.9010	18.9829	6085.0303
199	C	7	18568.6610	8.2931	16080.7350
200	O	7	11779.8430	18.9839	6084.6616
201	C	7	18568.4840	8.2933	16080.5070
202	Ca	7	8371.6509	27.1033	240.6630
203	O	7	11779.9020	18.9829	6085.0362
204	C	7	18568.6600	8.2931	16080.7350
205	O	7	11766.8980	19.1840	6011.7082
206	O	7	11766.6660	19.1843	6011.3835
207	O	7	11766.8980	19.1840	6011.7061
208	O	7	11766.6670	19.1843	6011.3865
209	O	7	11766.6680	19.1843	6011.3872
210	O	7	11766.8990	19.1840	6011.7055
211	O	8	11776.5940	19.1566	6029.6219
212	O	8	11776.5930	19.1566	6029.6228
213	O	8	11776.7820	19.1587	6029.1727
214	O	8	11776.7820	19.1587	6029.1748
215	O	8	11776.5960	19.1566	6029.6245
216	O	8	11776.7810	19.1587	6029.1717
217	Ca	8	8369.1507	27.0705	248.0019
218	Ca	8	8369.1496	27.0705	248.0016
219	O	8	11780.3970	18.9839	6085.2367
220	C	8	18572.7810	8.2865	16086.8320
221	O	8	11780.4410	18.9824	6085.7296
222	C	8	18572.5360	8.2864	16086.6200
223	Ca	8	8369.1562	27.0704	248.0489
224	Ca	8	8369.1566	27.0704	248.0495
225	Ca	8	8369.1499	27.0705	248.0017
226	O	8	11780.4410	18.9824	6085.7329
227	C	8	18572.5380	8.2864	16086.6220

228	O	8	11780.3960	18.9839	6085.2376
229	C	8	18572.7800	8.2865	16086.8310
230	O	8	11780.4410	18.9824	6085.7328
231	C	8	18572.5370	8.2864	16086.6210
232	Ca	8	8369.1560	27.0704	248.0489
233	O	8	11780.3970	18.9839	6085.2394
234	C	8	18572.7800	8.2865	16086.8310
235	O	8	11776.4390	19.1500	6031.4424
236	O	8	11776.4510	19.1498	6031.5214
237	O	8	11776.4380	19.1500	6031.4418
238	O	8	11776.4500	19.1498	6031.5206
239	O	8	11776.4380	19.1500	6031.4387
240	O	8	11776.4500	19.1498	6031.5163
241	O	9	11769.0140	19.1131	6035.0787
242	O	9	11769.0140	19.1131	6035.0779
243	O	9	11768.9060	19.1127	6035.0970
244	O	9	11768.9080	19.1127	6035.0943
245	O	9	11769.0140	19.1131	6035.0796
246	O	9	11768.9070	19.1127	6035.0969
247	Ca	9	8373.2194	26.8628	314.3694
248	O	9	11781.4560	18.9067	6109.4467
249	C	9	18568.8860	8.2407	16096.6750
250	O	9	11781.4030	18.9077	6109.0854
251	C	9	18568.9920	8.2408	16096.7540
252	Ca	9	8373.1898	26.8631	314.2479
253	Ca	9	8373.1899	26.8631	314.2487
254	Ca	9	8373.2193	26.8628	314.3685
255	O	9	11781.4000	18.9077	6109.0845
256	C	9	18568.9900	8.2408	16096.7520
257	O	9	11781.4560	18.9067	6109.4431
258	C	9	18568.8840	8.2407	16096.6740
259	O	9	11781.4020	18.9077	6109.0834
260	C	9	18568.9920	8.2408	16096.7540
261	Ca	9	8373.2199	26.8628	314.3690
262	Ca	9	8373.1899	26.8631	314.2489
263	O	9	11781.4560	18.9067	6109.4465
264	C	9	18568.8850	8.2407	16096.6750
265	O	9	11770.6380	19.0183	6065.1585
266	O	9	11770.5540	19.0194	6064.7431
267	O	9	11770.5560	19.0194	6064.7432
268	O	9	11770.6370	19.0183	6065.1599
269	O	9	11770.5550	19.0194	6064.7436
270	O	9	11770.6390	19.0183	6065.1601
271	O	10	11782.3560	18.7522	6156.6856
272	O	10	11782.3570	18.7522	6156.6850
273	O	10	11782.2880	18.7532	6156.3188
274	O	10	11782.2870	18.7532	6156.3199

275	O	10	11782.3560	18.7522	6156.6876
276	O	10	11782.2860	18.7532	6156.3203
277	Ca	10	8398.4099	25.2263	830.5274
278	O	10	11799.5840	18.3784	6286.0572
279	C	10	18596.1120	8.0015	16195.6560
280	O	10	11799.6080	18.3779	6286.2279
281	C	10	18596.1400	8.0015	16195.6950
282	Ca	10	8398.4300	25.2259	830.6730
283	Ca	10	8398.4305	25.2259	830.6735
284	Ca	10	8398.4101	25.2263	830.5257
285	O	10	11799.6090	18.3779	6286.2283
286	C	10	18596.1360	8.0015	16195.6900
287	O	10	11799.5850	18.3784	6286.0572
288	C	10	18596.1110	8.0015	16195.6550
289	O	10	11799.6100	18.3779	6286.2277
290	C	10	18596.1380	8.0015	16195.6930
291	Ca	10	8398.4107	25.2263	830.5269
292	Ca	10	8398.4297	25.2259	830.6745
293	O	10	11799.5850	18.3784	6286.0600
294	C	10	18596.1130	8.0015	16195.6570
295	O	10	11806.0730	18.0523	6390.3842
296	O	10	11806.0800	18.0529	6390.2213
297	O	10	11806.0800	18.0529	6390.2213
298	O	10	11806.0720	18.0523	6390.3831
299	O	10	11806.0810	18.0529	6390.2241
300	O	10	11806.0730	18.0523	6390.3845
		Σ	3738295.7255	5611.0245	2054988.3835

Table S4. Vibrational energy (E_j^{vib}), entropy (S_j^{vib}) and free energy (F_j^{vib}) at T = 300 K of the layers forming the (10.4) slab of calcite. The slab is composed by 10 layers (*l* = 1, …, 10, where *l* = 1 is the surface layer) both in the region 1 and 2. Here, only the atoms of the region 1, which are allowed to relax according to the GULP strategy, are reported. The percentage contribution of each layer to the vibrational energy (E=100× E_l^{vib}/Σ), entropy (S=100× S_l^{vib}/Σ) and free energy (F=100× F_l^{vib}/Σ) of the slab is also reported.

layer	E_l^{vib} (J/mol)	S_l^{vib} (J/mol/K)	F_l^{vib} (J/mol)	E (%)	S (%)	F (%)
1	373328.9800	621.8446	186775.6100	9.9866	11.0825	9.0889
2	375025.3200	563.2087	206062.7000	10.0320	10.0375	10.0274
3	373712.3300	558.4650	206172.8300	9.9969	9.9530	10.0328
4	373911.1900	557.5773	206637.9900	10.0022	9.9372	10.0554
5	373554.6400	557.1530	206408.7500	9.9926	9.9296	10.0443
6	373716.8700	556.9692	206626.1100	9.9970	9.9263	10.0549
7	373520.2000	556.5994	206540.4000	9.9917	9.9197	10.0507
8	373652.1800	555.8850	206886.6900	9.9953	9.9070	10.0675
9	373578.7700	552.8561	207721.9600	9.9933	9.8530	10.1082
10	374295.2400	530.4663	215155.3400	10.0125	9.4540	10.4699
Σ	3738295.7200	5611.0245	2054988.3800	100.0000	100.0000	100.0000