Supporting Information

A theoretical study on spontaneous dipole alignment in ice structures

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Table S1: $\langle\mu_x\rangle$, $\langle\mu_y\rangle$ and $\langle\mu_z\rangle$ and the corresponding standard errors of the mean (SEM) at $T_g = 150K$.

T_s (K)	$\langle\mu_x\rangle$ (eÅ)	$SEM_{\langle\mu_x\rangle}$	$\langle\mu_y\rangle$ (eÅ)	$SEM_{\langle\mu_y\rangle}$	$\langle\mu_z\rangle$ (eÅ)	$SEM_{\langle\mu_z\rangle}$
10	-0.00019	0.00405	0.00394	0.00407	-0.01212	0.00312
20	0.00095	0.00674	0.00227	0.00570	-0.01369	0.00180
30	-0.00002	0.00301	-0.00092	0.00249	-0.01219	0.00209
40	0.00114	0.00411	-0.00056	0.00516	-0.01192	0.00240
50	0.00398	0.00353	0.00128	0.00245	-0.01484	0.00300
60	0.00415	0.00525	-0.00101	0.00443	-0.01448	0.00249
70	0.00820	0.00436	-0.00231	0.00616	-0.00710	0.00242
80	0.00162	0.00255	0.00224	0.00220	-0.00811	0.00192
90	0.00054	0.00429	-0.00184	0.00584	-0.00252	0.00285
100	-0.00427	0.00537	0.00202	0.00360	-0.00785	0.00221
110	-0.00859	0.00486	-0.00010	0.00411	-0.00581	0.00368
120	-0.00112	0.00412	-0.00090	0.00434	-0.00190	0.00182
130	-0.00151	0.00242	0.00295	0.00247	0.00276	0.00182
140	0.00099	0.00533	0.00667	0.00206	0.00670	0.00383

Table S2: $\langle\mu_x\rangle$, $\langle\mu_y\rangle$ and $\langle\mu_z\rangle$ and the corresponding standard errors of the mean (SEM) at $T_g = 300K$.

T_s (K)	$\langle\mu_x\rangle$ (eÅ)	$SEM_{\langle\mu_x\rangle}$	$\langle\mu_y\rangle$ (eÅ)	$SEM_{\langle\mu_y\rangle}$	$\langle\mu_z\rangle$ (eÅ)	$SEM_{\langle\mu_z\rangle}$
10	0.00279	0.00279	0.00190	0.00308	-0.02179	0.00186
20	-0.00828	0.00439	-0.00462	0.00449	-0.01389	0.00245
30	-0.00223	0.00232	-0.00347	0.00222	-0.01442	0.00126
40	-0.00576	0.00529	-0.00754	0.00677	-0.01234	0.00181
50	0.00649	0.00523	-0.00038	0.00540	-0.00851	0.00286
60	-0.01037	0.00590	-0.00575	0.00432	-0.00996	0.00311
70	-0.00740	0.00283	-0.00096	0.00584	-0.00755	0.00444
80	-0.00299	0.00258	-0.00048	0.00306	-0.00509	0.00183
90	-0.00008	0.00321	-0.00156	0.00544	-0.00511	0.00219
100	0.00420	0.00573	-0.00134	0.00427	-0.00665	0.00304
110	-0.00029	0.00561	-0.00200	0.00451	-0.00379	0.00213
120	-0.00088	0.00569	-0.00160	0.00661	-0.00002	0.00310
130	-0.00189	0.00348	0.00307	0.00316	-0.00121	0.00139
140	0.00904	0.00815	-0.00510	0.00455	-0.00128	0.00335

Table S3: $\langle \mu_z \rangle$, $\langle \mu_z \rangle / \mu$, E_{cal}, d and V_s and the corresponding standard errors of the mean (SEM) at $T_g = 150K$.

T_s (K)	$\langle \mu_z \rangle$ $(e\text{Å})$	$SEM_{\langle \mu_z \rangle}$	$\langle \mu_z \rangle / \mu$	E_{cal} $(\times 10^{+8}\ Vm^{-1})$	d (Å)	SEM_d	V_s (V)	SEM_{V_s}
10	-0.01212	0.00312	-0.02525	-6.89	43.7199	2.4489	-3.0559	0.7773
20	-0.01369	0.00180	-0.02853	-7.79	41.5309	1.8680	-3.2188	0.4132
30	-0.01219	0.00209	-0.02540	-6.93	40.9429	1.3235	-2.7630	0.4411
40	-0.01192	0.00240	-0.02483	-6.78	39.9724	1.9057	-2.5880	0.5258
50	-0.01484	0.00300	-0.03091	-8.44	41.7626	1.7620	-3.4220	0.7152
60	-0.01448	0.00249	-0.03017	-8.23	38.9102	1.5497	-3.0648	0.5180
70	-0.00710	0.00242	-0.01479	-4.04	34.6209	1.1685	-1.3731	0.4987
80	-0.00811	0.00192	-0.01691	-4.61	37.0365	1.2818	-1.7749	0.4281
90	-0.00252	0.00285	-0.00526	-1.44	37.1652	1.7803	-0.4102	0.6147
100	-0.00785	0.00221	-0.01637	-4.47	37.1326	1.8506	-1.6003	0.4387
110	-0.00581	0.00368	-0.01210	-3.30	35.4604	2.3107	-1.3720	0.8134
120	-0.00190	0.00182	-0.00397	-1.08	35.0269	1.5527	-0.3740	0.3864
130	0.00276	0.00182	0.00574	1.57	32.2863	0.9403	0.6721	0.2854
140	0.00670	0.00383	0.01396	3.81	29.8822	1.5673	1.2578	0.7015

Table S4: $\langle \mu_z \rangle$, $\langle \mu_z \rangle / \mu$, E_{cal}, d and V_s and the corresponding standard errors of the mean (SEM) at $T_g = 300K$.

T_s (K)	$\langle \mu_z \rangle$ $(e\text{Å})$	$SEM_{\langle \mu_z \rangle}$	$\langle \mu_z \rangle / \mu$	E_{cal} $(\times 10^{+8}\ Vm^{-1})$	d (Å)	SEM_d	V_s (V)	SEM_{V_s}
10	-0.02179	0.00186	-0.04540	-12.39	39.3780	2.1509	-4.9724	0.5493
20	-0.01389	0.00245	-0.02893	-7.90	39.0883	1.4890	-3.0890	0.5750
30	-0.01442	0.00126	-0.03004	-8.20	34.6728	1.2078	-2.8315	0.2835
40	-0.01234	0.00181	-0.02572	-7.02	35.1525	1.6598	-2.5738	0.4548
50	-0.00851	0.00286	-0.01774	-4.84	33.8206	1.8568	-1.4980	0.5583
60	-0.00996	0.00311	-0.02076	-5.67	33.2558	1.5506	-1.9240	0.6029
70	-0.00755	0.00444	-0.01574	-4.30	32.3657	1.8175	-1.3323	0.8428
80	-0.00509	0.00183	-0.01060	-2.89	33.7683	0.9003	-1.0132	0.3608
90	-0.00511	0.00219	-0.01065	-2.91	30.2608	1.7188	-0.8355	0.3806
100	-0.00665	0.00304	-0.01387	-3.78	31.2509	1.8551	-1.0053	0.5761
110	-0.00379	0.00213	-0.00789	-2.15	30.0533	0.8136	-0.6695	0.3873
120	-0.00002	0.00310	-0.00004	-0.01	30.6580	1.4151	0.0280	0.5319
130	-0.00121	0.00139	-0.00251	-0.69	30.1717	0.7288	-0.2437	0.2578
140	-0.00128	0.00335	-0.00268	-0.73	29.5324	0.9654	-0.2363	0.6131

Table S5: Results for Layer 1 at $T_g = 150K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	0.00173	0.00349	0.00360	0.98	149	8	7.287	0.408	0.08417	0.14173
20	-0.00546	0.00270	-0.01138	-3.11	165	7	6.922	0.311	-0.22151	0.10725
30	-0.00246	0.00146	-0.00513	-1.40	162	5	6.824	0.221	-0.11210	0.05117
40	-0.00110	0.00194	-0.00229	-0.62	162	7	6.662	0.318	-0.04700	0.07333
50	-0.00295	0.00305	-0.00615	-1.68	166	7	6.960	0.294	-0.09861	0.11837
60	-0.00415	0.00356	-0.00864	-2.36	174	6	6.485	0.258	-0.15663	0.12468
70	0.00641	0.00255	0.01336	3.65	172	4	5.770	0.195	0.21362	0.08855
80	0.00375	0.00168	0.00782	2.13	167	4	6.173	0.214	0.11279	0.05907
90	0.00833	0.00237	0.01735	4.74	158	6	6.194	0.297	0.27528	0.08206
100	0.00339	0.00165	0.00706	1.93	168	5	6.189	0.308	0.11779	0.05368
110	0.00615	0.00321	0.01281	3.50	170	4	5.910	0.385	0.15419	0.09283
120	0.00814	0.00287	0.01697	4.63	155	8	5.838	0.259	0.25347	0.08631
130	0.01146	0.00197	0.02388	6.52	166	3	5.381	0.157	0.33180	0.06092
140	0.01218	0.00305	0.02538	6.93	172	5	4.980	0.261	0.34300	0.08922

Table S6: Results for Layer 2 at $T_g = 150K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	-0.01460	0.00699	-0.03042	-8.30	76	7	7.287	0.408	-0.50147	0.25042
20	-0.01941	0.00512	-0.04045	-11.04	97	7	6.922	0.311	-0.72950	0.18753
30	-0.01946	0.00165	-0.04055	-11.07	88	3	6.824	0.221	-0.74915	0.05751
40	-0.01830	0.00578	-0.03813	-10.41	86	6	6.662	0.318	-0.64204	0.21520
50	-0.02313	0.00405	-0.04819	-13.15	94	6	6.960	0.294	-0.91990	0.17711
60	-0.02528	0.00524	-0.05267	-14.37	78	8	6.485	0.258	-0.87807	0.18630
70	-0.01489	0.00431	-0.03102	-8.47	94	5	5.770	5.770	-0.47396	0.13076
80	-0.01454	0.00284	-0.03030	-8.27	95	3	6.173	6.173	-0.52240	0.10719
90	-0.01063	0.00504	-0.02215	-6.05	93	5	6.194	0.297	-0.32700	0.18260
100	-0.01489	0.00409	-0.03102	-8.47	94	7	6.189	0.308	-0.51849	0.13844
110	-0.01985	0.00544	-0.04137	-11.29	89	6	5.910	0.385	-0.64147	0.18652
120	-0.01245	0.00368	-0.02594	-7.08	101	5	5.838	0.259	-0.40526	0.11531
130	-0.00875	0.00276	-0.01822	-4.97	95	3	5.381	0.157	-0.23471	0.08408
140	0.00408	0.00467	0.00849	2.32	101	4	4.980	0.261	0.12825	0.14131

Table S7: Results for Layer 3 at $T_g = 150K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	-0.00685	0.00733	-0.01427	-3.90	74	5	7.287	0.408	-0.28946	0.28474
20	-0.01204	0.00521	-0.02510	-6.85	80	6	6.922	0.311	-0.47540	0.20762
30	-0.01223	0.00368	-0.02548	-6.95	74	2	6.824	0.221	-0.45225	0.14593
40	-0.01697	0.00416	-0.03536	-9.65	73	5	6.662	0.318	-0.64397	0.15662
50	-0.01434	0.00631	-0.02988	-8.15	72	5	6.960	0.294	-0.52954	0.24347
60	-0.01555	0.00490	-0.03240	-8.84	75	3	6.485	0.258	-0.53564	0.16700
70	-0.00143	0.00839	-0.00299	-0.81	70	5	5.770	5.770	-0.01907	0.28876
80	-0.01607	0.00347	-0.03348	-9.14	81	2	6.173	6.173	-0.58773	0.13211
90	-0.00052	0.00437	-0.00108	-0.29	88	4	6.194	0.297	0.00619	0.15474
100	-0.01006	0.00498	-0.02096	-5.72	86	5	6.189	0.308	-0.32386	0.18361
110	-0.00568	0.00594	-0.01183	-3.23	82	4	5.910	0.385	-0.23321	0.22167
120	-0.00569	0.00391	-0.01186	-3.24	87	3	5.838	0.259	-0.20818	0.13929
130	0.00161	0.00395	0.00336	0.92	83	2	5.381	0.157	0.06353	0.14177
140	-0.00382	0.00890	-0.00797	-0.22	83	3	4.980	0.261	-0.05528	0.27518

Table S8: Results for Layer 4 at $T_g = 150K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	-0.02550	0.00714	-0.05314	-14.50	78	4	7.287	0.408	-1.13482	0.36844
20	-0.00994	0.00482	-0.02071	-5.65	75	6	6.922	0.311	-0.42161	0.19157
30	-0.01044	0.00490	-0.02176	-5.94	75	3	6.824	0.221	-0.38711	0.17606
40	-0.01210	0.00685	-0.02522	-6.88	69	4	6.662	0.318	-0.40377	0.25364
50	-0.02202	0.00604	-0.04588	-12.52	77	5	6.960	0.294	-0.82002	0.23649
60	-0.02023	0.00785	-0.04216	-11.51	76	6	6.485	0.258	-0.74897	0.27251
70	-0.01481	0.00510	-0.03086	-8.42	75	4	5.770	5.770	-0.49182	0.16651
80	-0.01428	0.00526	-0.02976	-8.12	68	3	6.173	6.173	-0.50103	0.18787
90	-0.01108	0.00517	-0.02308	-6.30	77	4	6.194	0.297	-0.35963	0.16979
100	-0.01098	0.00461	-0.02288	-6.25	74	5	6.189	0.308	-0.42537	0.18534
110	-0.00987	0.00717	-0.02056	-5.61	77	4	5.910	0.385	-0.35972	0.24651
120	-0.00278	0.00722	-0.00580	-1.58	75	5	5.838	0.259	-0.06186	0.22898
130	0.00240	0.00375	0.00501	1.37	73	2	5.381	0.157	0.08244	0.11618
140	0.00461	0.00745	0.00960	2.62	69	3	4.980	0.261	0.16333	0.20137

Table S9: Results for Layer 5 at $T_g = 150K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	-0.01274	0.00746	-0.02654	-7.24	83	7	7.287	0.408	-0.58949	0.33050
20	-0.03030	0.00625	-0.06313	-17.23	56	9	6.922	0.311	-1.14255	0.23615
30	-0.01853	0.00350	-0.03862	-10.54	65	4	6.824	0.221	-0.66472	0.13279
40	-0.01402	0.00592	-0.02921	-7.97	73	7	6.662	0.318	-0.49675	0.22542
50	-0.02060	0.00549	-0.04293	-11.72	61	5	6.960	0.294	-0.82858	0.22495
60	-0.01059	0.00576	-0.02207	-6.02	61	4	6.485	0.258	-0.32755	0.21739
70	-0.01742	0.00354	-0.03630	-9.91	62	4	5.770	5.770	-0.56167	0.11179
80	-0.00683	0.00385	-0.01423	-3.88	59	3	6.173	6.173	-0.21586	0.13376
90	-0.00742	0.00726	-0.01547	-4.22	54	4	6.194	0.297	-0.19663	0.25134
100	-0.01892	0.00691	-0.03942	-10.76	52	5	6.189	0.308	-0.59440	0.22199
110	-0.00792	0.00946	-0.01650	-4.50	55	7	5.910	0.385	-0.37416	0.28824
120	0.00460	0.00629	0.00958	2.61	58	4	5.838	0.259	0.19566	0.21179
130	0.00226	0.00419	0.00472	1.29	58	3	5.381	0.157	0.09306	0.13280
140	0.01889	0.00388	0.03935	10.74	52	3	4.980	0.261	0.54564	0.12083

Table S10: Results for Layer 6 at $T_g = 150K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	-0.03734	0.00462	-0.07780	-21.23	41	4	7.287	0.408	-1.60041	0.24376
20	-0.01889	0.00935	-0.03936	-10.74	27	3	6.922	0.311	-0.73176	0.35389
30	-0.02613	0.00546	-0.05444	-14.86	36	2	6.824	0.221	-0.96718	0.20857
40	-0.01875	0.01080	-0.03908	-10.67	37	4	6.662	0.318	-0.72362	0.39414
50	-0.01708	0.01251	-0.03558	-9.71	30	4	6.960	0.294	-0.68107	0.47928
60	-0.03068	0.01132	-0.06392	-17.44	37	6	6.485	0.258	-1.02768	0.40251
70	-0.03189	0.01127	-0.06644	-18.13	27	3	5.770	5.770	-1.10021	0.38281
80	-0.02050	0.00476	-0.04271	-11.66	30	2	6.173	6.173	-0.74372	0.16845
90	-0.01590	0.00960	-0.03314	-9.04	30	3	6.194	0.297	-0.51416	0.33005
100	-0.01654	0.00752	-0.03447	-9.41	27	3	6.189	0.308	-0.53303	0.23928
110	-0.01635	0.01094	-0.03407	-9.30	27	3	5.910	0.385	-0.51555	0.28657
120	-0.01846	0.00909	-0.03845	-10.50	25	2	5.838	0.259	-0.63651	0.32920
130	-0.00148	0.00753	-0.00308	-0.84	24	2	5.381	0.157	0.00629	0.24203
140	0.00296	0.00802	0.00617	1.69	23	2	4.980	0.261	0.12603	0.23794

Table S11: Results for Layer 1 at $T_g = 300K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times 10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	-0.00620	0.00323	-0.01292	-3.53	151	5	6.563	0.358	-0.25586	0.12285
20	-0.00469	0.00227	-0.00977	-2.67	176	5	6.515	0.248	-0.18874	0.09180
30	-0.00126	0.00148	-0.00262	-0.71	165	3	5.779	0.201	0.10930	0.04666
40	-0.00206	0.00287	-0.00429	-1.17	171	6	5.859	0.277	-0.08783	0.09923
50	0.00825	0.00232	0.01720	4.69	163	9	5.637	0.309	0.24647	0.07008
60	0.00421	0.00270	0.00878	2.40	170	7	5.543	0.258	0.13815	0.08260
70	0.00655	0.00289	0.01366	3.73	171	9	5.394	0.303	0.19329	0.09458
80	0.00660	0.00178	0.01374	3.75	173	3	5.628	0.150	0.19771	0.02515
90	0.01025	0.00222	0.02136	5.83	173	7	5.043	0.286	0.30025	0.07184
100	0.00881	0.00202	0.01835	5.01	162	6	5.208	0.309	0.25241	0.05734
110	0.00960	0.00177	0.02001	5.46	168	6	5.009	0.136	0.26899	0.04823
120	0.01031	0.00306	0.02148	5.86	169	4	5.110	0.236	0.28861	0.08843
130	0.01270	0.00152	0.02645	7.22	171	3	5.029	0.121	0.35072	0.04403
140	0.00990	0.00311	0.02062	5.63	171	6	4.922	0.161	0.27225	0.08429

Table S12: Results for Layer 2 at $T_g = 300K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times 10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	-0.01876	0.00368	-0.03910	-10.67	92	8	6.563	0.358	-0.71589	0.15842
20	-0.02218	0.00462	-0.04622	-12.61	81	5	6.515	0.248	-0.80217	0.16797
30	-0.01911	0.00195	-0.03981	-10.87	89	3	5.779	0.201	-0.45264	0.06884
40	-0.01816	0.00546	-0.03785	-10.33	101	5	5.859	0.277	-0.60304	0.18184
50	-0.01226	0.00707	-0.02555	-6.97	99	4	5.637	0.309	-0.32104	0.21695
60	-0.01653	0.00400	-0.03444	-9.40	105	5	5.543	0.258	-0.55432	0.14564
70	-0.01028	0.00304	-0.02143	-5.85	95	5	5.394	0.303	-0.32705	0.09571
80	-0.01472	0.00335	-0.03068	-8.37	99	3	5.628	0.150	-0.40953	0.13542
90	-0.01358	0.00426	-0.02830	-7.73	94	3	5.043	0.286	-0.39594	0.13815
100	-0.01333	0.00514	-0.02776	-7.58	98	4	5.208	0.309	-0.33433	0.16524
110	-0.00989	0.00536	-0.02061	-5.62	100	5	5.009	0.136	-0.28010	0.15466
120	-0.00031	0.00571	-0.00065	0.18	97	5	5.110	0.236	-0.00240	0.18167
130	-0.00857	0.00268	-0.01786	-4.87	101	2	5.029	0.121	-0.43760	0.06667
140	-0.01043	0.00463	-0.02174	-5.93	96	5	4.922	0.161	-0.28302	0.14305

Table S13: Results for Layer 3 at $T_g = 300K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times 10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	-0.02728	0.00516	-0.05684	-15.51	85	3	6.563	0.358	-1.04882	0.22777
20	-0.01687	0.00580	-0.03515	-9.59	69	7	6.515	0.248	-0.62190	0.21594
30	-0.02222	0.00199	-0.04629	-12.63	78	3	5.779	0.201	-0.70777	0.05666
40	-0.01483	0.00375	-0.03090	-8.43	84	6	5.859	0.277	-0.49775	0.12263
50	-0.01679	0.00787	-0.03499	-9.55	85	4	5.637	0.309	-0.51652	0.25291
60	-0.01637	0.00489	-0.03411	-9.31	83	5	5.543	0.258	-0.52225	0.16754
70	-0.02202	0.01050	-0.04588	-12.52	78	6	5.394	0.303	-0.68908	0.35994
80	-0.00703	0.00273	-0.01465	-3.99	80	2	5.628	0.150	-0.22828	0.09005
90	-0.00979	0.00469	-0.02041	-5.57	82	5	5.043	0.286	-0.28382	0.15004
100	-0.00909	0.00494	-0.01894	-5.17	83	3	5.208	0.309	-0.23454	0.15367
110	-0.00601	0.00497	-0.01252	-3.42	83	3	5.009	0.136	-0.17897	0.15326
120	-0.00479	0.00637	-0.00998	-2.72	77	3	5.110	0.236	-0.11114	0.18978
130	-0.00498	0.00387	-0.01038	-2.83	83	3	5.029	0.121	-0.15507	0.12017
140	-0.00406	0.00494	-0.00846	-2.31	79	4	4.922	0.161	-0.12575	0.14225

Table S14: Results for Layer 4 at $T_g = 300K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	-0.02647	0.00347	-0.05516	-15.05	74	6	6.563	0.358	-1.00595	0.14989
20	-0.01306	0.00500	-0.02721	-7.43	72	3	6.515	0.248	-0.48486	0.18039
30	-0.01530	0.00335	-0.03188	-8.70	74	2	5.779	0.201	-0.49489	0.09619
40	-0.01949	0.00670	-0.04061	-11.08	65	5	5.859	0.277	-0.70978	0.24255
50	-0.01512	0.00459	-0.03150	-8.60	75	4	5.637	0.309	-0.47258	0.14684
60	-0.01754	0.00688	-0.03654	-9.97	71	5	5.543	0.258	-0.53385	0.21079
70	-0.01787	0.00810	-0.03724	-10.16	72	4	5.394	0.303	-0.52963	0.25272
80	-0.00854	0.00451	-0.01778	-4.85	70	2	5.628	0.150	-0.26269	0.15565
90	-0.02015	0.00449	-0.04198	-11.46	71	3	5.043	0.286	-0.58919	0.11894
100	-0.01784	0.00511	-0.03718	-10.15	75	3	5.208	0.309	-0.45789	0.13204
110	0.00494	-0.03008	-0.03008	-8.21	72	5	5.009	0.136	-0.40062	0.13149
120	-0.00727	0.00335	-0.01516	-4.14	72	4	5.110	0.236	-0.19449	0.07977
130	-0.00663	0.00260	-0.01382	-3.77	70	2	5.029	0.121	-0.18851	0.07331
140	-0.00177	0.00725	-0.00369	-1.01	72	4	4.922	0.161	-0.06107	0.20604

Table S15: Results for Layer 5 at $T_g = 300K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	-0.03813	0.00742	-0.07945	-21.68	66	8	6.563	0.358	-1.34684	0.24318
20	-0.02301	0.00692	-0.04794	-13.09	72	7	6.515	0.248	-0.82356	0.22697
30	-0.02092	0.00382	-0.04359	-11.90	63	3	5.779	0.201	-0.69487	0.12394
40	-0.00905	0.00331	-0.01886	-5.15	51	6	5.859	0.277	-0.32659	0.11806
50	-0.02367	0.00571	-0.04932	-13.46	56	5	5.637	0.309	-0.71419	0.16931
60	-0.01421	0.00703	-0.02961	-8.08	51	4	5.543	0.258	-0.46393	0.21356
70	-0.01183	0.00657	-0.02466	-6.73	54	5	5.394	0.303	-0.35807	0.20622
80	-0.00794	0.00504	-0.01654	-4.51	53	3	5.628	0.150	-0.23902	0.16565
90	-0.01258	0.00681	-0.02622	-7.16	57	3	5.043	0.286	-0.34725	0.21531
100	-0.01324	0.00931	-0.02759	-7.53	59	4	5.208	0.309	-0.32347	0.27683
110	-0.00938	0.00481	-0.01954	-5.33	55	5	5.009	0.136	-0.27780	0.14840
120	-0.00263	0.00714	-0.00547	-1.49	56	4	5.110	0.236	-0.04438	0.17885
130	-0.00874	0.00340	-0.01822	-4.97	52	3	5.029	0.121	-0.25351	0.09805
140	-0.00589	0.00706	-0.01228	-3.35	56	3	4.922	0.161	-0.16474	0.22269

Table S16: Results for Layer 6 at $T_g = 300K$.

T_s (K)	$\langle\mu_z\rangle$ $(e\text{Å})$	$SEM_{\langle\mu_z\rangle}$	$\langle\mu_z\rangle/\mu$	E_{cal} $(\times10^{+8}\ Vm^{-1})$	N_W	SEM_{N_W}	d_l (Å)	SEM_{d_l}	$V(d_l)$ (V)	$SEM_{V(d_l)}$
10	-0.05193	0.00808	-0.10820	-29.53	33	3	6.563	0.358	-1.97875	0.33216
20	-0.03700	0.00910	-0.07709	-21.04	30	3	6.515	0.248	-1.37175	0.35143
30	-0.03149	0.00328	-0.06562	-17.91	31	1	5.779	0.201	-0.95764	0.12880
40	-0.01616	0.00990	-0.03367	-9.19	27	4	5.859	0.277	-0.55169	0.33576
50	-0.00472	0.01973	-0.00984	-2.69	22	3	5.637	0.309	-0.14167	0.60411
60	-0.01756	0.01292	-0.03658	-9.98	21	1	5.543	0.258	-0.63808	0.42067
70	-0.00825	0.00891	-0.01718	-4.69	30	3	5.394	0.303	-0.17762	0.27992
80	-0.01943	0.00716	-0.04049	-11.05	26	2	5.628	0.150	-0.55452	0.23193
90	-0.00111	0.01413	-0.00232	-0.63	24	3	5.043	0.286	0.00876	0.40814
100	-0.02300	0.00553	-0.04792	-13.08	24	2	5.208	0.309	-0.71633	0.21722
110	-0.01071	0.01378	-0.02231	-6.09	22	3	5.009	0.136	-0.33903	0.38649
120	-0.01715	0.01201	-0.03574	-9.75	29	4	5.110	0.236	-0.52230	0.34660
130	-0.02038	0.00781	-0.04246	-11.59	23	1	5.029	0.121	-0.57465	0.22471
140	-0.01468	0.01102	-0.03059	-8.35	27	2	4.922	0.161	-0.41392	0.31909

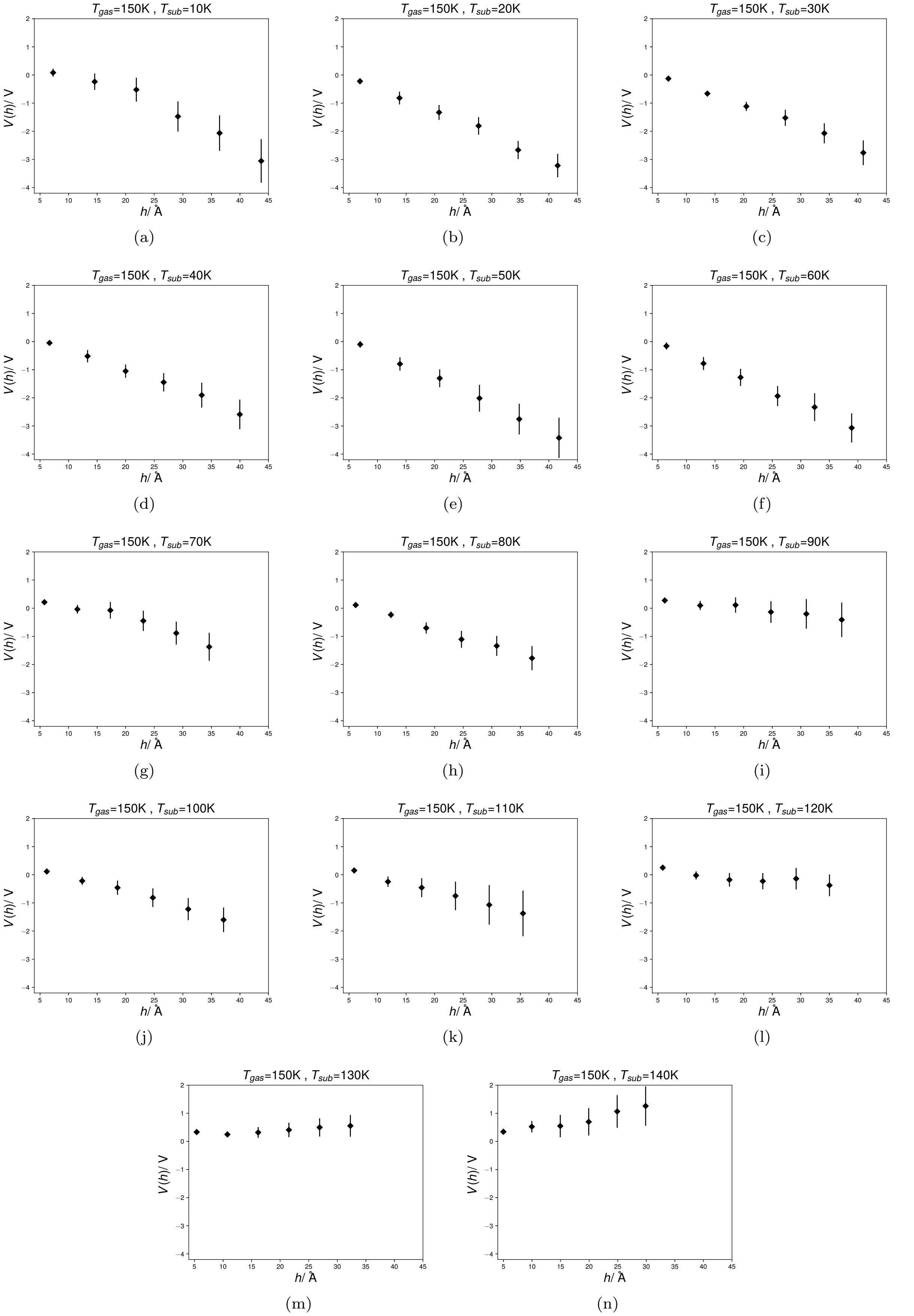

Figure S1: The height dependence of the potential $V(h)$ at T_g=150 K and T_s between 10 K and 140 K.

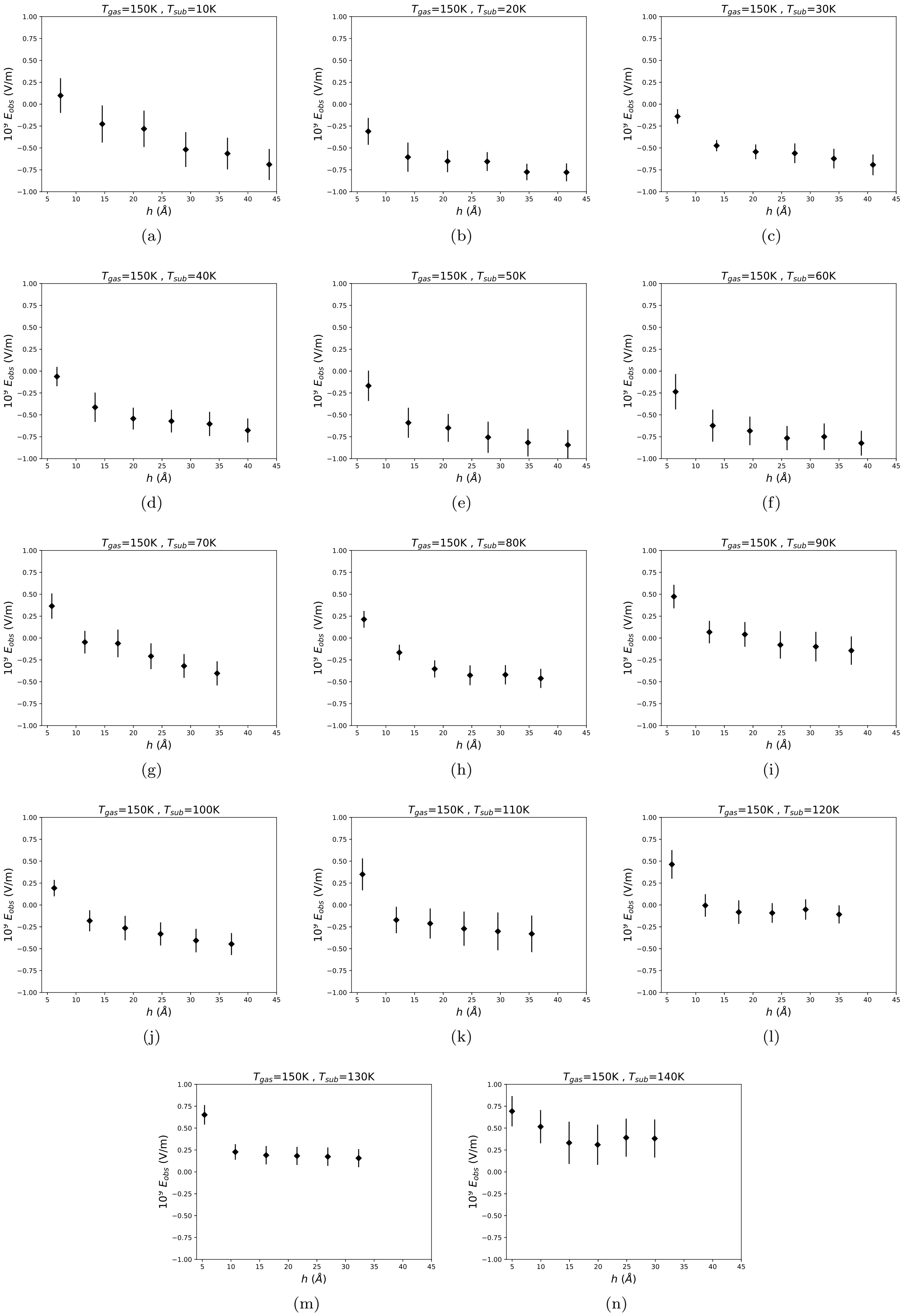

Figure S2: The height dependence of the electric field at T_g=150 K and T_s between 10 K and 140 K.

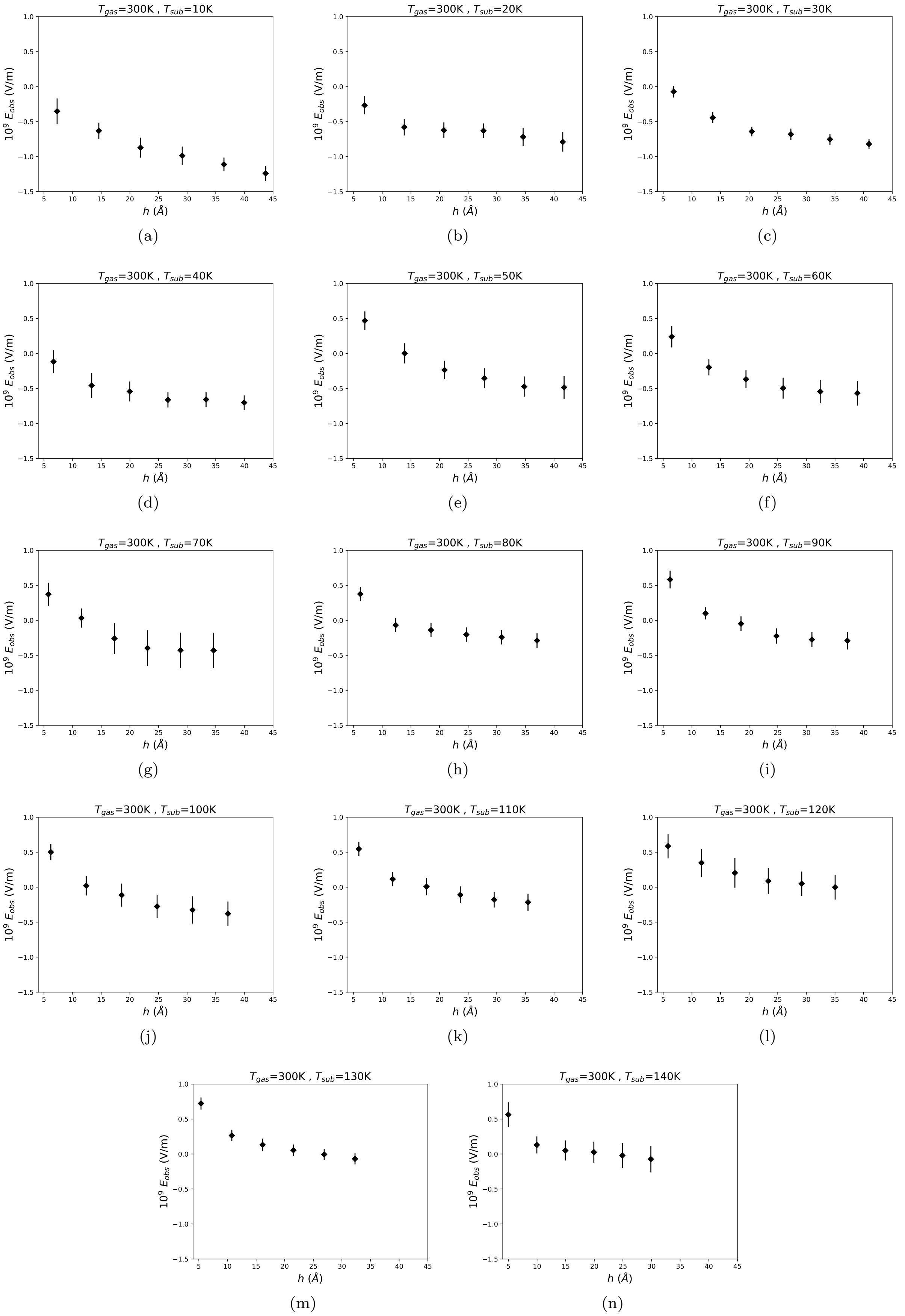

Figure S3: The height dependence of the electric field at T_g=150 K and T_s between 10 K and 140 K.