Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Isoconfigurational molecular dynamics study of structural effect on the kinetics of crystal growth of hexagonal ice I_h. Supplementary information

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July 13, 2012

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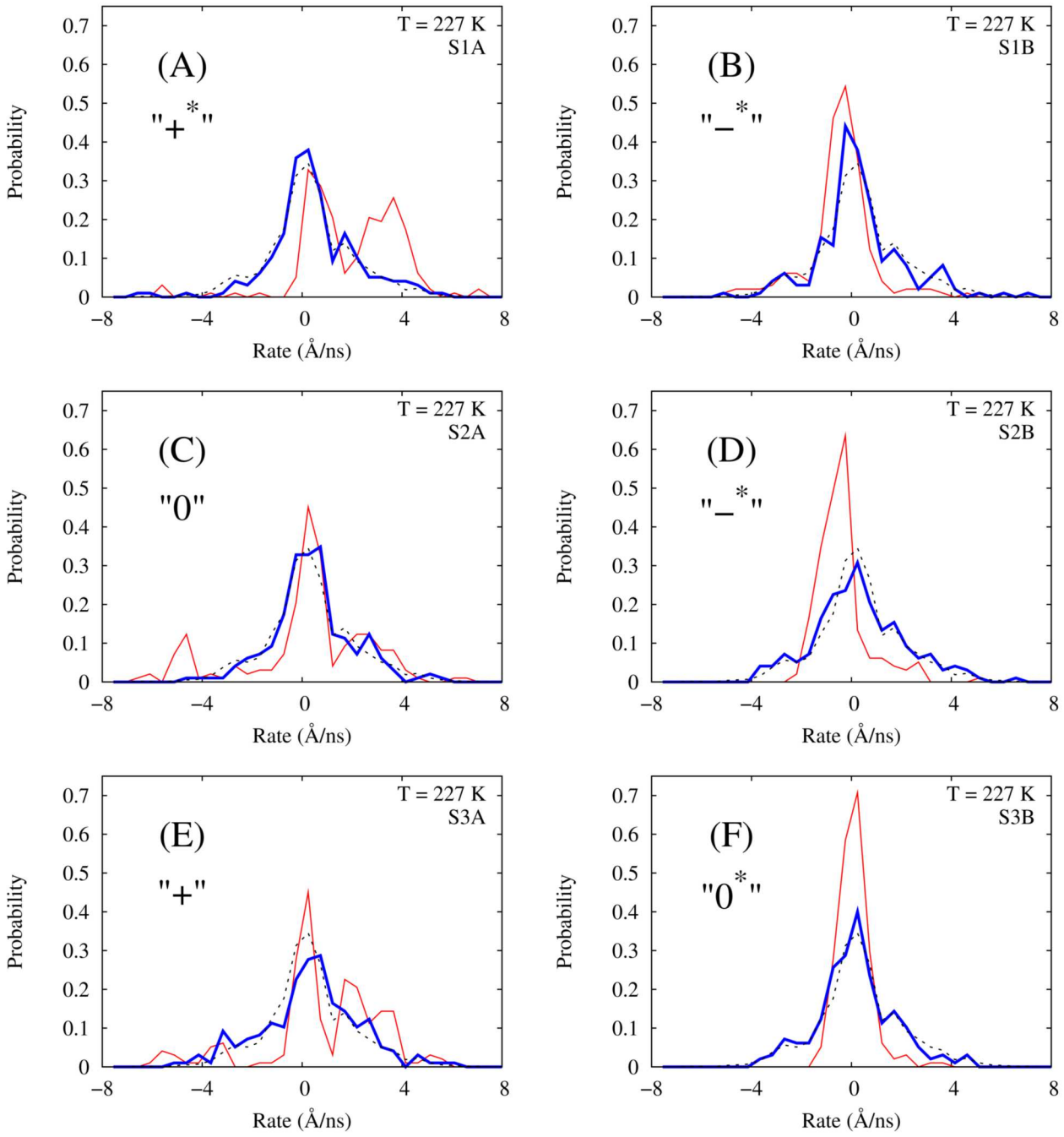

Figure 1: Probability distributions of 200 isoconfigurational ice growth rates (based on 1 ns time windows) for the six interfaces at $T = 227$ K: (A) S1A, (B) S1B, (C) S2A, (D) S2B, (E) S3A, (F) S3B. The rate distributions are shown at the beginning (thin red lines) and at the end (blue thick lines) of the simulation trajectories. For comparison, the dashed lines show the average rate distribution typical to the specific temperature, taken as the distributions averaged over six isoconfigurational runs. The temperature, system, and interface for a specific isoconfigurational simulation are indicated in the top right corner of the plots. The notation used for a specific propensity is also shown in each graph in quote marks. Configurations with the same naming at different temperatures are different.

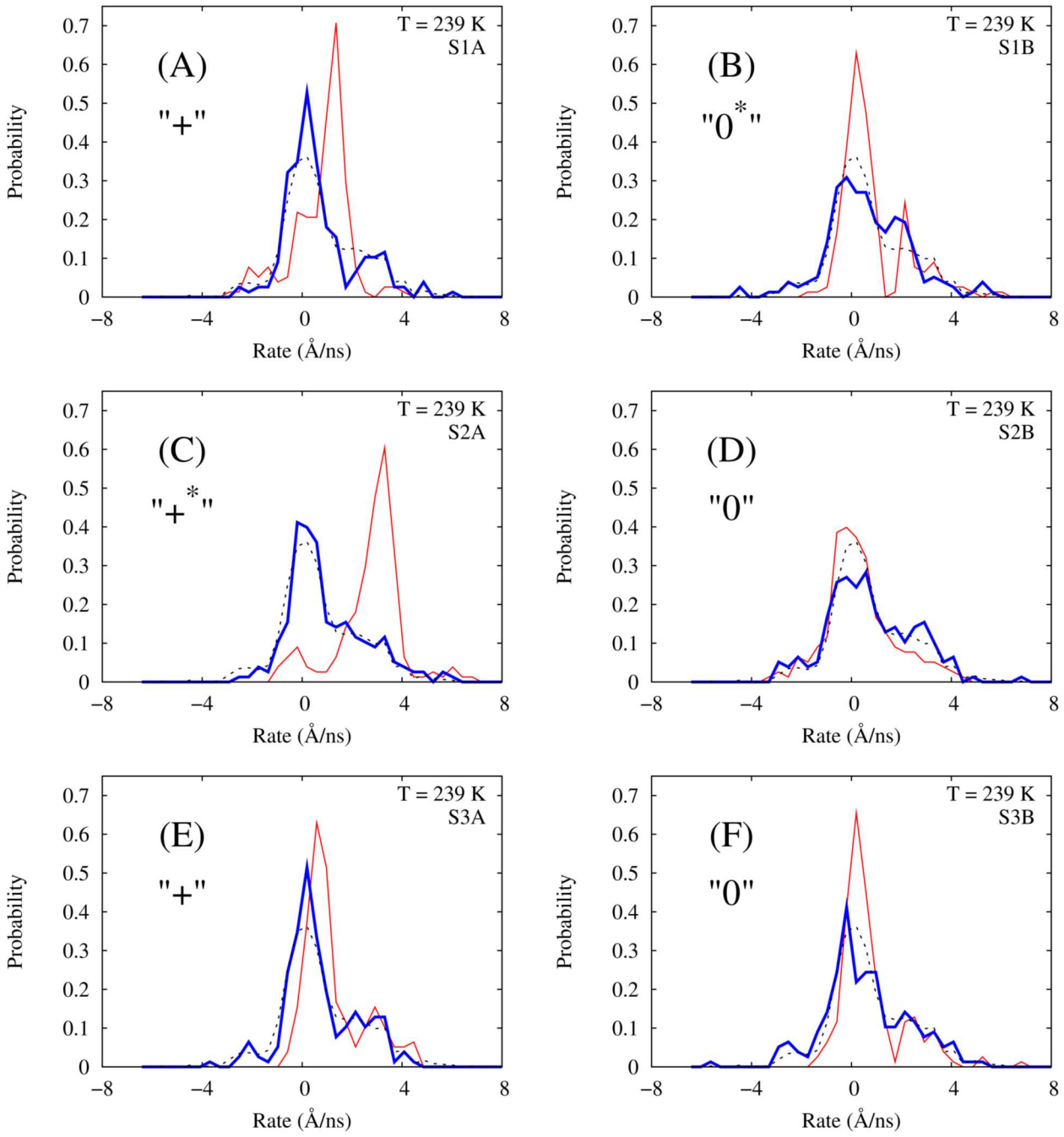

Figure 2: Probability distributions of 200 isoconfigurational ice growth rates (based on 1 ns time windows) for the six interfaces at $T = 239$ K: (A) S1A, (B) S1B, (C) S2A, (D) S2B, (E) S3A, (F) S3B. The rate distributions are shown at the beginning (thin red lines) and at the end (blue thick lines) of the simulation trajectories. For comparison, the dashed lines show the average rate distribution typical to the specific temperature, taken as the distributions averaged over six isoconfigurational runs. The temperature, system, and interface for a specific isoconfigurational simulation are indicated in the top right corner of the plots. The notation used for a specific propensity is also shown in each graph in quote marks. Configurations with the same naming at different temperatures are different.

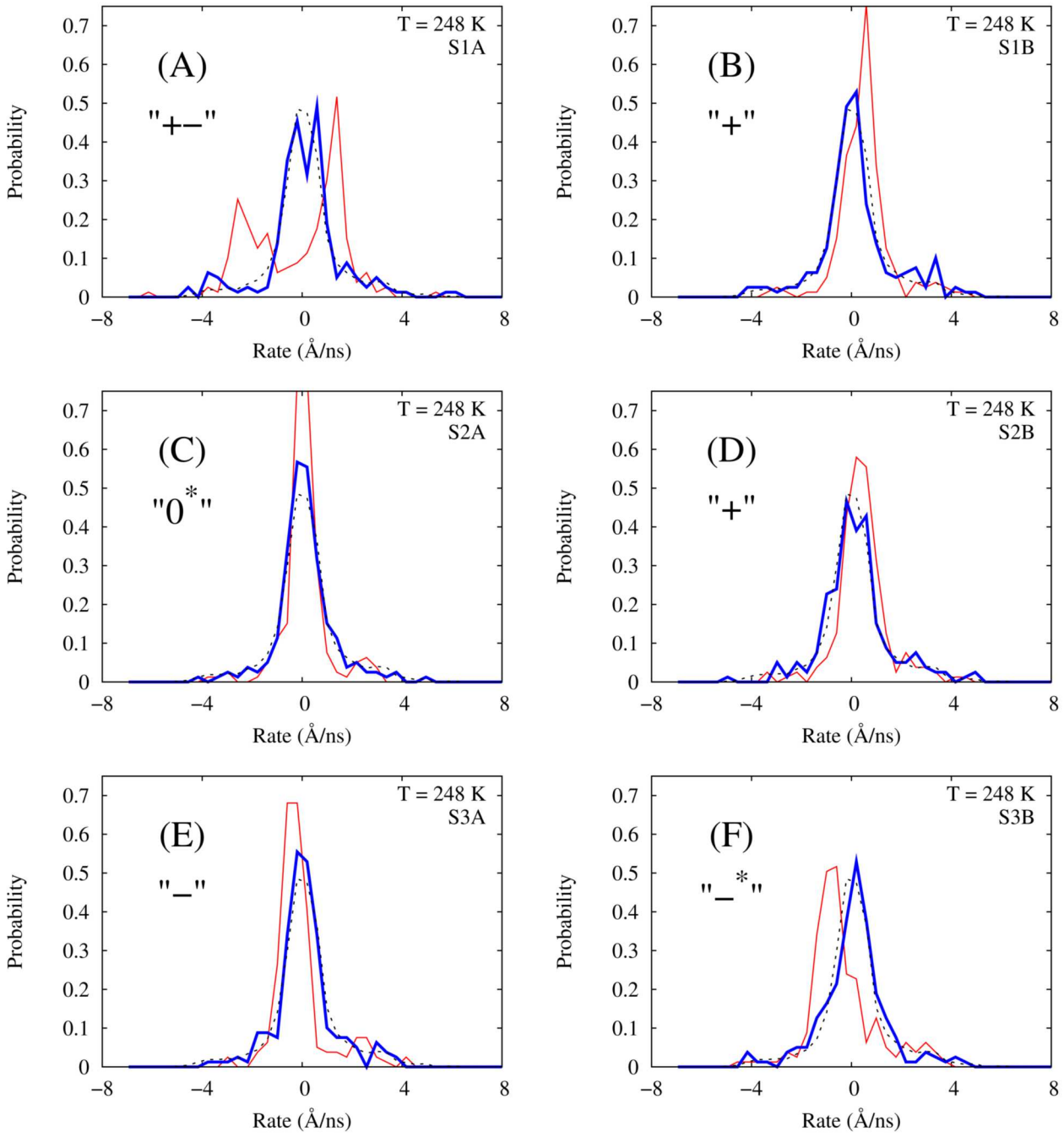

Figure 3: Probability distributions of 200 isoconfigurational ice growth rates (based on 1 ns time windows) for the six interfaces at $T = 248$ K: (A) S1A, (B) S1B, (C) S2A, (D) S2B, (E) S3A, (F) S3B. The rate distributions are shown at the beginning (thin red lines) and at the end (blue thick lines) of the simulation trajectories. For comparison, the dashed lines show the average rate distribution typical to the specific temperature, taken as the distributions averaged over six isoconfigurational runs. The temperature, system, and interface for a specific isoconfigurational simulation are indicated in the top right corner of the plots. The notation used for a specific propensity is also shown in each graph in quote marks. Configurations with the same naming at different temperatures are different.

Table 1: Statistics of the growth rate distributions obtained at the three temperatures for six different initial configurations in this work, as well as for the total rate sets for each temperature during the first 1 ns of the simulations. The mean value, the standard deviation (STD), the skewness of the distributions, as well as their kurtosis are shown. The last column gives the interface growth propensities assigned on the basis of visual examination using the notation explained in the main text.

Temperature (K)	Rate set	Mean (A/ns)	STD (A/ns)	Skewness	Kurtosis	Growth propensity
227	S1A	1.87	1.98	-0.77	2.25	+*
	S1B	-0.47	1.32	-0.28	2.98	-
	S2A	0.16	2.44	-0.68	0.51	0
	S2B	-0.36	1.01	1.78	4.90	-*
	S3A	0.81	2.29	-0.84	1.00	+
	S3B	0.12	0.69	1.53	5.90	0*
	Total	0.35	1.92	-0.16	1.55	
239	S1A	0.77	1.14	-0.70	1.28	+
	S1B	0.84	1.32	1.36	1.66	0*
	S2A	2.73	1.34	-0.56	1.58	+*
	S2B	0.32	1.39	0.56	0.65	0
	S3A	1.23	1.19	1.11	0.33	+
	S3B	0.79	1.27	1.54	2.95	0
	Total	1.11	1.49	0.56	0.32	
248	S1A	-0.13	1.83	-0.29	-0.55	+-
	S1B	0.50	1.05	0.47	4.12	+
	S2A	0.10	0.94	0.01	4.31	0*
	S2B	0.43	1.04	0.40	3.52	+
	S3A	-0.07	1.07	1.63	3.62	-
	S3B	-0.39	1.35	0.68	1.51	-*
	Total	0.07	1.29	0.04	1.68	

Table 2: Statistics of the growth rate distributions obtained at the three temperatures for six different initial configurations in this work, as well as for the total rate sets for each temperature during the last 1 ns of the simulations. The mean value, the standard deviation (STD), the skewness of the distributions, as well as their kurtosis are shown. The variations of the statistical values indicate the uncertainty of the values in uncorrelated sets.

Temperature (K)	Rate set	Mean (A/ns)	STD (A/ns)	Skewness	Kurtosis
227	S1A	0.51	1.86	0.34	3.95
	S1B	0.38	1.81	0.98	3.34
	S2A	0.42	1.64	0.22	0.83
	S2B	0.33	1.86	0.37	0.30
	S3A	0.31	1.98	-0.09	0.22
	S3B	0.20	1.53	0.21	0.55
	Total	0.36	1.78	0.34	1.74
239	S1A	0.68	1.44	1.01	1.13
	S1B	0.66	1.64	0.26	0.96
	S2A	0.93	1.54	0.89	0.68
	S2B	0.78	1.77	0.65	1.20
	S3A	0.71	1.43	0.32	0.06
	S3B	0.58	1.71	0.12	0.45
	Total	0.72	1.59	0.51	0.96
248	S1A	0.11	1.53	0.04	3.08
	S1B	0.19	1.49	0.32	1.46
	S2A	0.11	1.14	0.42	3.36
	S2B	0.21	1.39	0.48	2.22
	S3A	0.12	1.18	0.35	1.86
	S3B	0.08	1.34	0.00	2.06
	Total	0.14	1.35	0.26	2.57

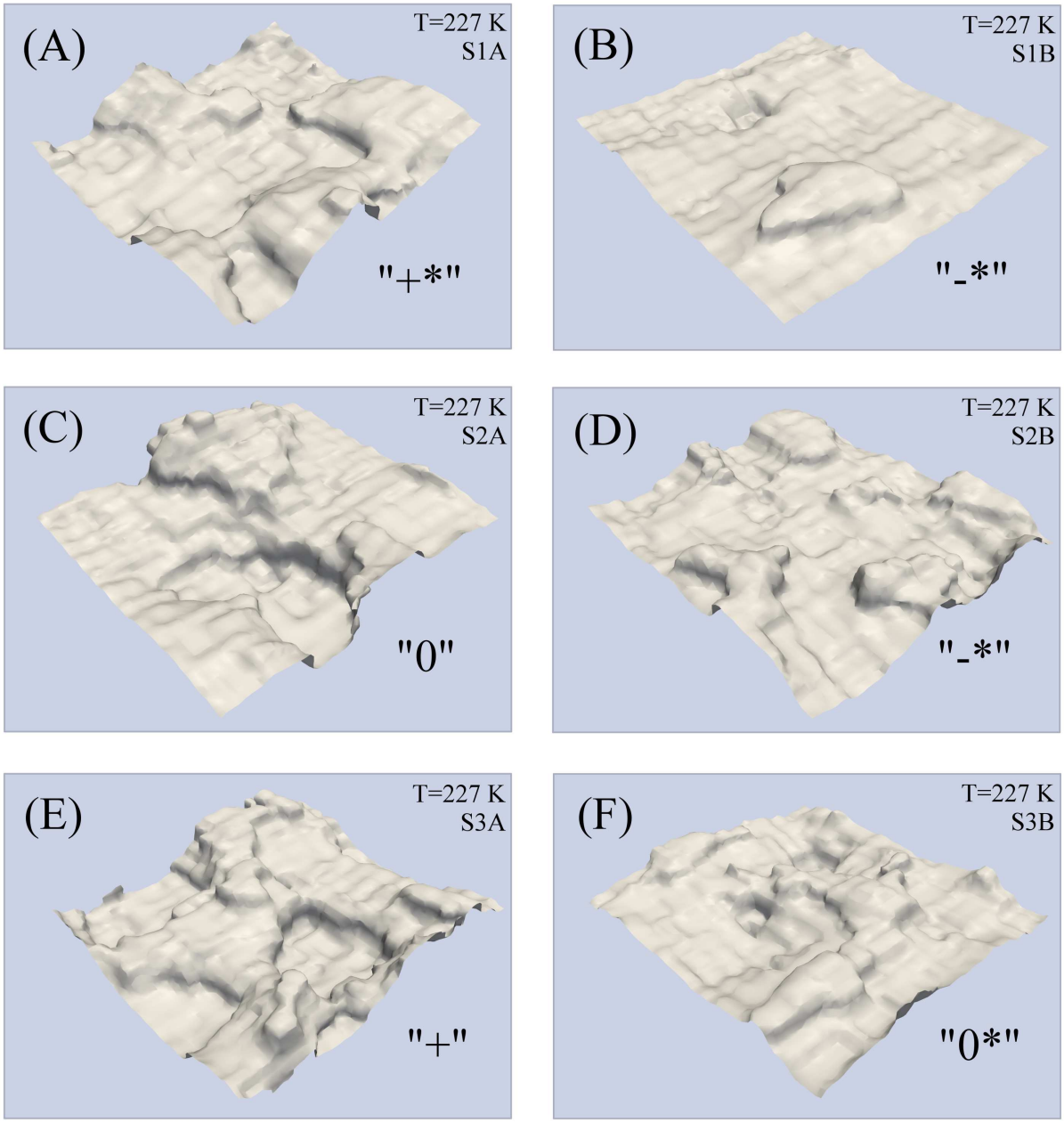

Figure 4: Interfaces surfaces based on structural order parameter averaged over first 10 ps of simulation and over 200 isoconfigurational trajectories for the six interfaces at $T = 227$ K: (A) S1A, (B) S1B, (C) S2A, (D) S2B, (E) S3A, (F) S3B. The ice phase is below the surface and the liquid water is above the surface. The surface dimensions are approximately 27×31 Å^2 and the thickness of one ice layer is about 3.7 Å. The surfaces correspond to the rate distributions shown in SI Fig. 1. The notation used for a specific propensity is also shown in each graph in quote marks. Configurations with the same naming at different temperatures are different.

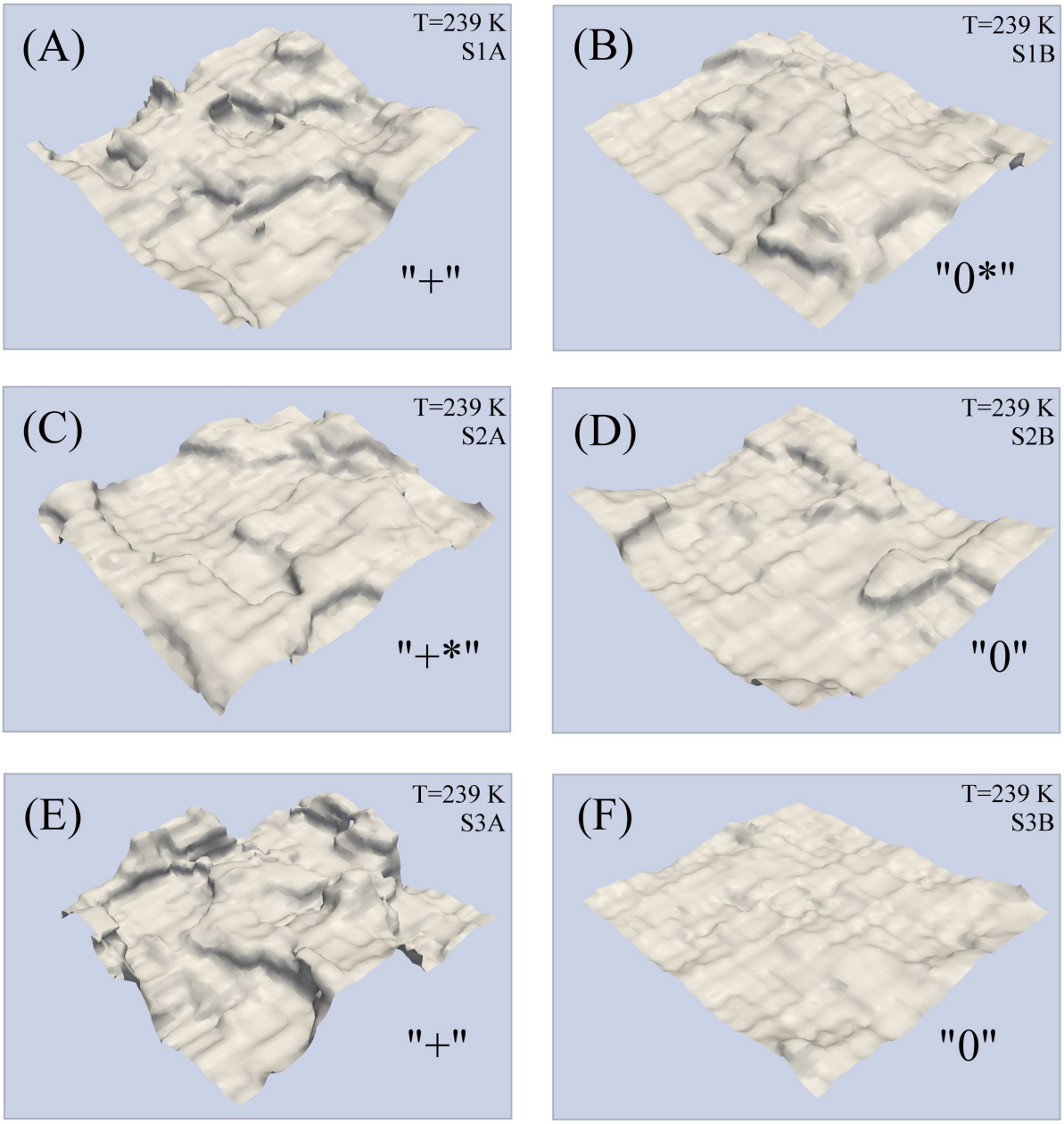

Figure 5: Interfaces surfaces based on structural order parameter averaged over first 10 ps of simulation and over 200 isoconfigurational trajectories for the six interfaces at $T = 239$ K: (A) S1A, (B) S1B, (C) S2A, (D) S2B, (E) S3A, (F) S3B. The ice phase is below the surface and the liquid water is above the surface. The surface dimensions are approximately 27×31 Å^2 and the thickness of one ice layer is about 3.7 Å. The surfaces correspond to the rate distributions shown in SI Fig. 2. The notation used for a specific propensity is also shown in each graph in quote marks. Configurations with the same naming at different temperatures are different.

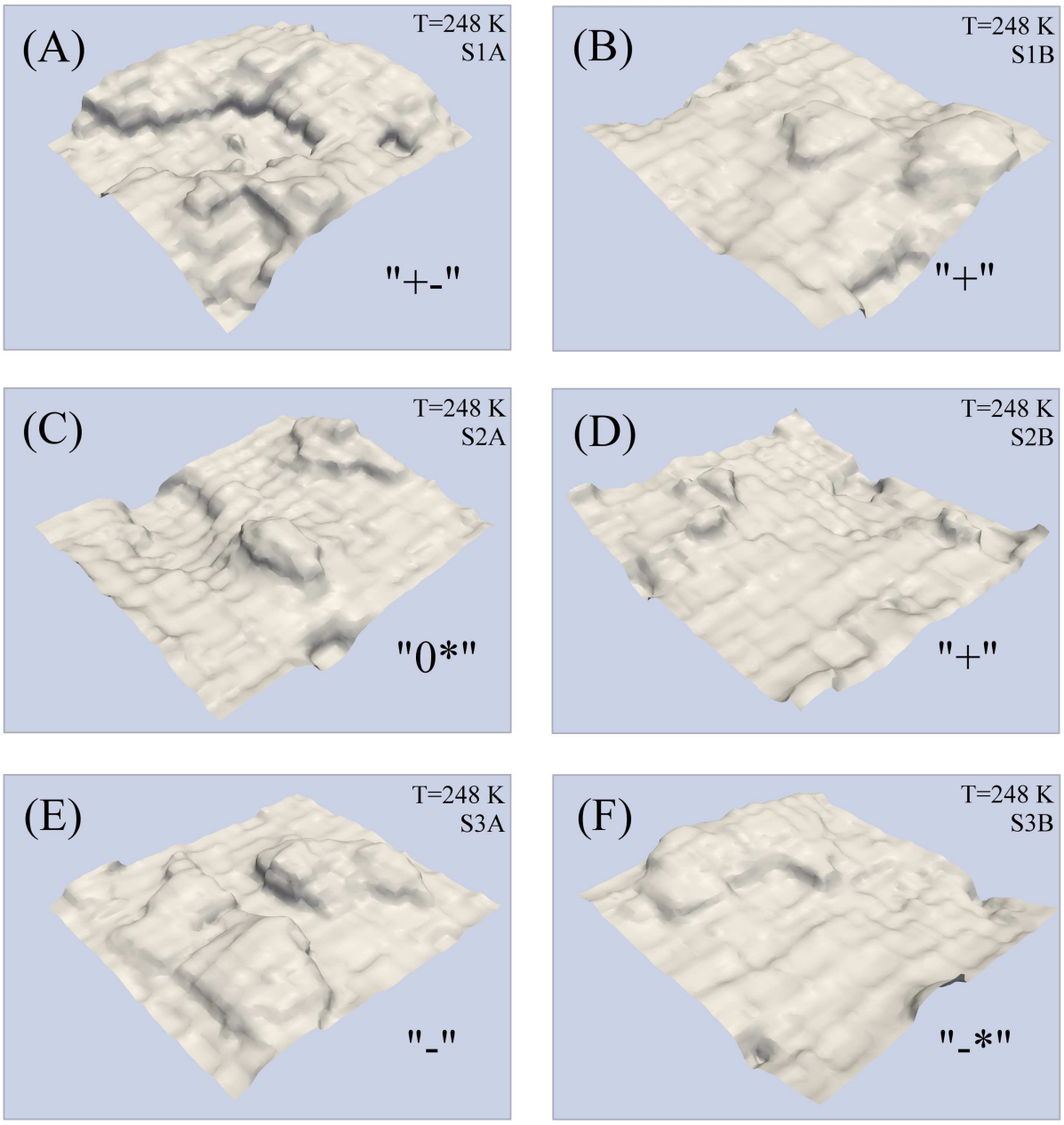

Figure 6: Interfaces surfaces based on structural order parameter averaged over first 10 ps of simulation and over 200 isoconfigurational trajectories for the six interfaces at $T = 248$ K: (A) S1A, (B) S1B, (C) S2A, (D) S2B, (E) S3A, (F) S3B. The ice phase is below the surface and the liquid water is above the surface. The surface dimensions are approximately 27×31 Å^2 and the thickness of one ice layer is about 3.7 Å. The surfaces correspond to the rate distributions shown in SI Fig. 3. The notation used for a specific propensity is also shown in each graph in quote marks. Configurations with the same naming at different temperatures are different.