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Article

Effect of Graphene on Ice Polymorph

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Table S1. Cubicity of the nucleation stage in each simulation trajectory.

Substrate	***Graphene***	***O-Haeckelite***	***R-Haeckelite***	***Random***	***Homo***
Ice nucleation	25.7	37.3	41.8	37.0	51.6
	20.0	54.4	28.8	60.9	52.7
	7.1	49.3	66.5	6.9	58.3
	24.5	24.9	39.9	69.7	35.6
	54.6	26.4	11.9	38.2	61.2
	30.7	48.4	56.1	48.4	55.0
	34.1	32.5	36.7	31.4	62.3
	46.9	43.5	70.2	58.8	52.6
	62.2	51.6	44.7	72.3	44.7
	37.5	53.5	50.2	39.0	58.7
	49.3	46.9	48.4	63.2	44.5
	29.0	34.4	8.5	26.1	53.7
	32.1	11.3	54.0	38.2	42.4
	5.0	32.2	65.0	50.7	51.0
	26.6	30.7	45.1	57.9	57.4
	27.6	51.5	30.2	66.6	58.0
	39.3	64.5	17.1	31.2	58.8
	27.8	35.7	40.2	57.4	47.2
	2.7	28.2	37.7	51.3	56.4
	18.9	50.0	20.7	35.8	45.8
Cubicity / %	13.0	49.5	41.8	37.6	49.3
	22.8	43.1	63.7	23.4	55.6
	16.2	57.3	36.2	61.2	54.9
	35.8	37.1	37.1	42.0	55.6
	14.1	39.5	38.7	27.7	63.4

	34.7	41.2	20.3	37.2	29.7
	35.0	53.7	42.4	57.6	69.5
	41.7	59.9	66.3	28.5	57.9
	22.9	44.5	50.2	54.5	37.9
	7.5	31.9	32.1	31.3	56.1
	33.8	34.8	39.4	50.5	50.5
	52.0	56.1	51.1	16.3	53.1
	54.8	38.8	38.2	46.9	61.1
	5.1	22.0	40.8	8.4	52.5
	3.3	47.8	39.0	22.5	47.0
	50.5	35.8	53.1	18.2	60.5
	49.9	21.7	45.6	9.3	56.4
	10.2	54.7	60.0	62.5	57.5
	8.8	47.4	61.2	65.5	33.1
	23.3	22.5	44.8	60.9	51.7
Substrate	***Graphene***	***O-Haeckelite***	***R-Haeckelite***	***Random***	***Homo***
Freezing	53.9	64.6	65.2	59.9	54.6
Completely	68.1	43.0	52.0	67.9	62.5
	60.9	47.6	69.4	32.3	59.9
	54.9	55.6	55.7	61.4	64.8
	72.1	55.4	53.4	58.7	49.1
	46.2	56.9	50.4	53.1	65.1
	63.9	60.8	66.4	52.4	65.6
	49.0	59.7	73.9	66.7	61.3
	44.8	47.3	70.2	58.8	63.3
	30.2	41.4	59.4	50.7	55.9
	57.7	75.6	57.3	42.8	63.4
	47.3	36.6	50.8	54.3	58.8
	62.4	66.9	51.7	56.6	56.0
	48.6	45.8	51.6	58.2	63.9
	36.0	48.6	26.0	55.2	62.1
	61.9	52.5	45.9	53.5	61.1
	70.6	63.2	66.9	48.1	57.8
	59.2	47.3	52.7	67.0	57.5
	27.6	51.3	58.1	52.8	57.3
Cubicity / %	45.8	52.6	47.4	35.4	57.2
	73.2	67.7	66.6	72.4	54.5
	52.5	68.6	68.2	48.6	51.7
	60.2	65.4	65.0	66.2	63.9
	63.6	39.1	56.3	68.6	57.9
	26.1	59.9	42.9	51.1	54.2
	66.1	76.3	56.2	33.3	61.9

64.6	60.9	63.3	63.0	55.3
44.2	45.8	59.1	39.2	60.3
45.3	53.6	70.8	59.5	57.1
46.0	56.3	56.1	54.7	55.3
57.2	62.8	38.7	71.6	55.9
38.4	52.4	61.2	43.5	60.3
52.0	44.8	62.7	42.7	57.9
56.8	56.9	58.7	32.7	57.3
51.0	55.8	49.6	59.7	54.5
50.2	62.8	47.9	57.3	59.4
42.0	53.7	58.5	67.2	46.1
67.1	47.6	60.3	56.3	57.2
57.3	47.2	52.8	70.0	54.3
60.0	62.0	40.8	57.4	54.6

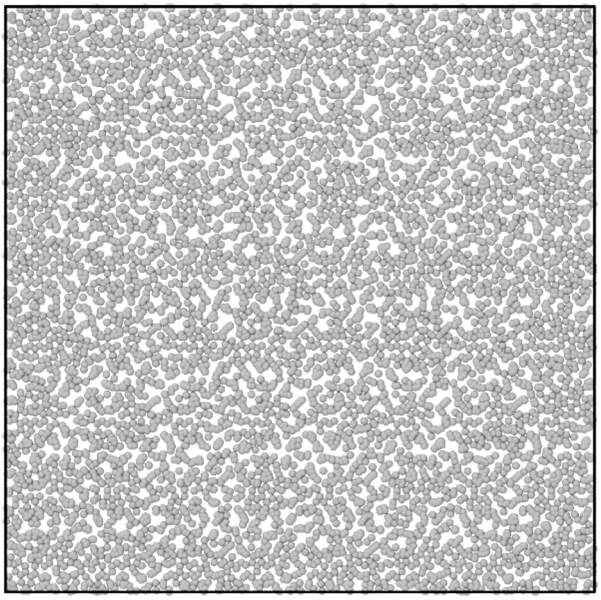

Figure S1. Surface morphology of 2-dimensional carbon substrate with all the carbon atoms randomly distributed, the *Random* system.

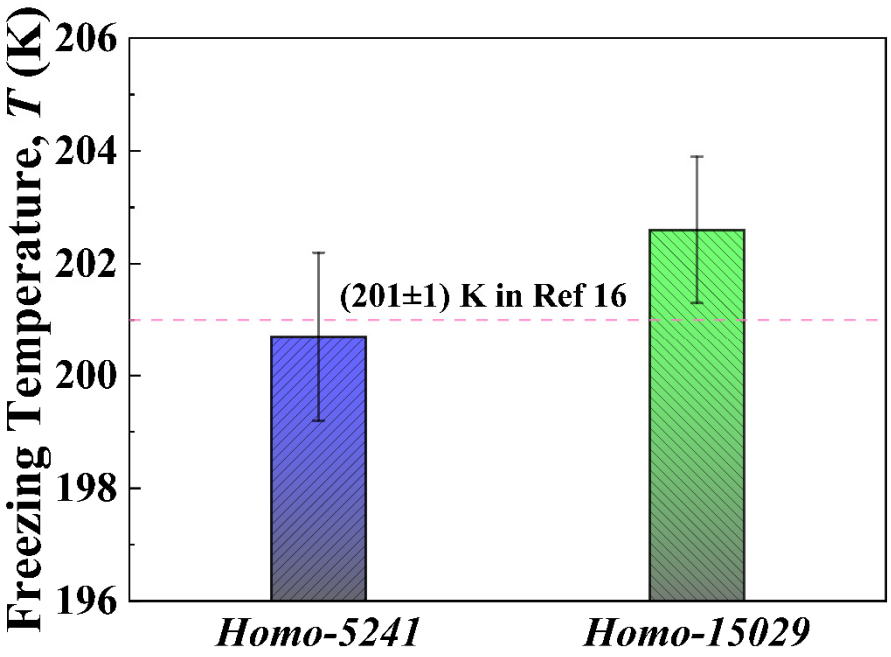

Figure S2. Freezing temperature in *Homo-5241* (5241 water molecules) and *Homo-15029* (15029 water molecules) systems by 20 independent MD trajectories.