Supplement of Atmos. Chem. Phys., 22, 10099–10114, 2022
https://doi.org/10.5194/acp-22-10099-2022-supplement

Atmospheric Chemistry and Physics
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EGU

Supplement of

Atomistic and coarse-grained simulations reveal increased ice nucleation activity on silver iodide surfaces in slit and wedge geometries

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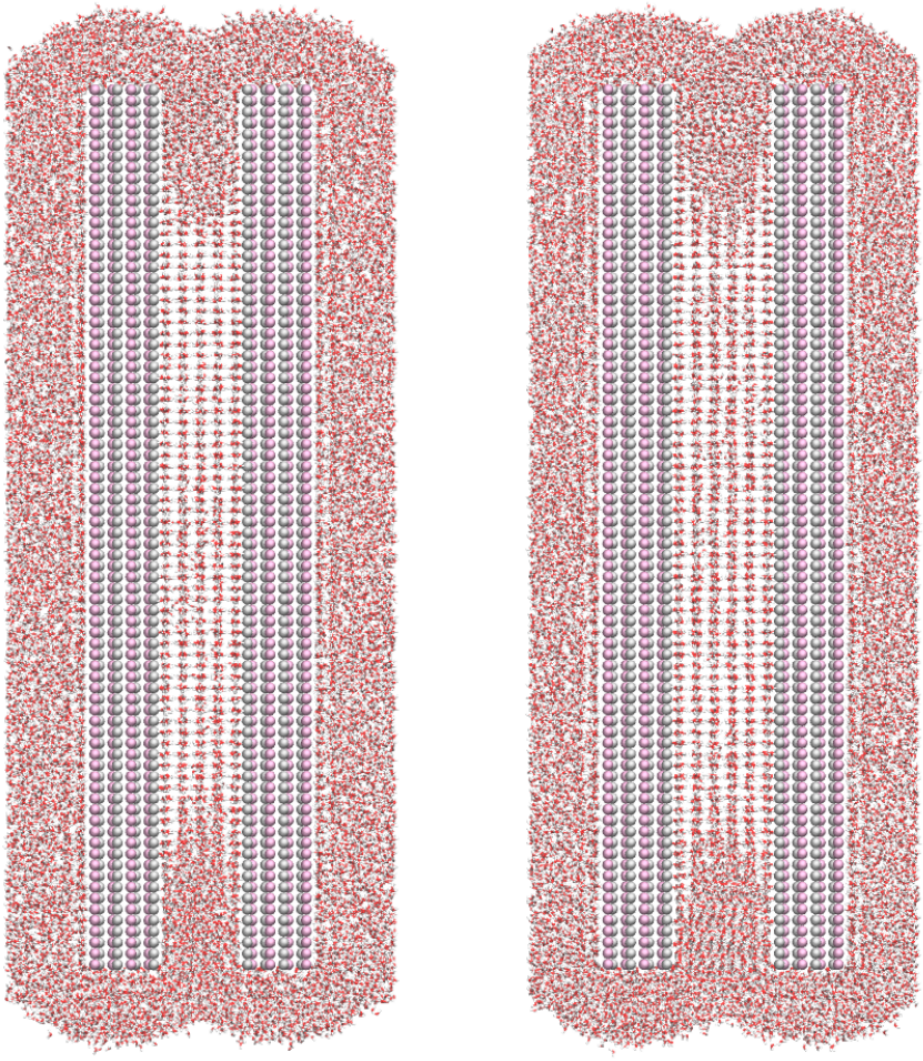

Figure S1. Snapshots of the final configurations of ice nucleation simulations at $T = 263$ K using the TIP4P/Ice water model in AgI slit systems with a gap width of 5 (left) and 6 (right) ice bilayers. Ag and I are shown in silver and pink, respectively, and water molecules are shown as red and white sticks. In both systems, ice cannot grow close to the slab edges.

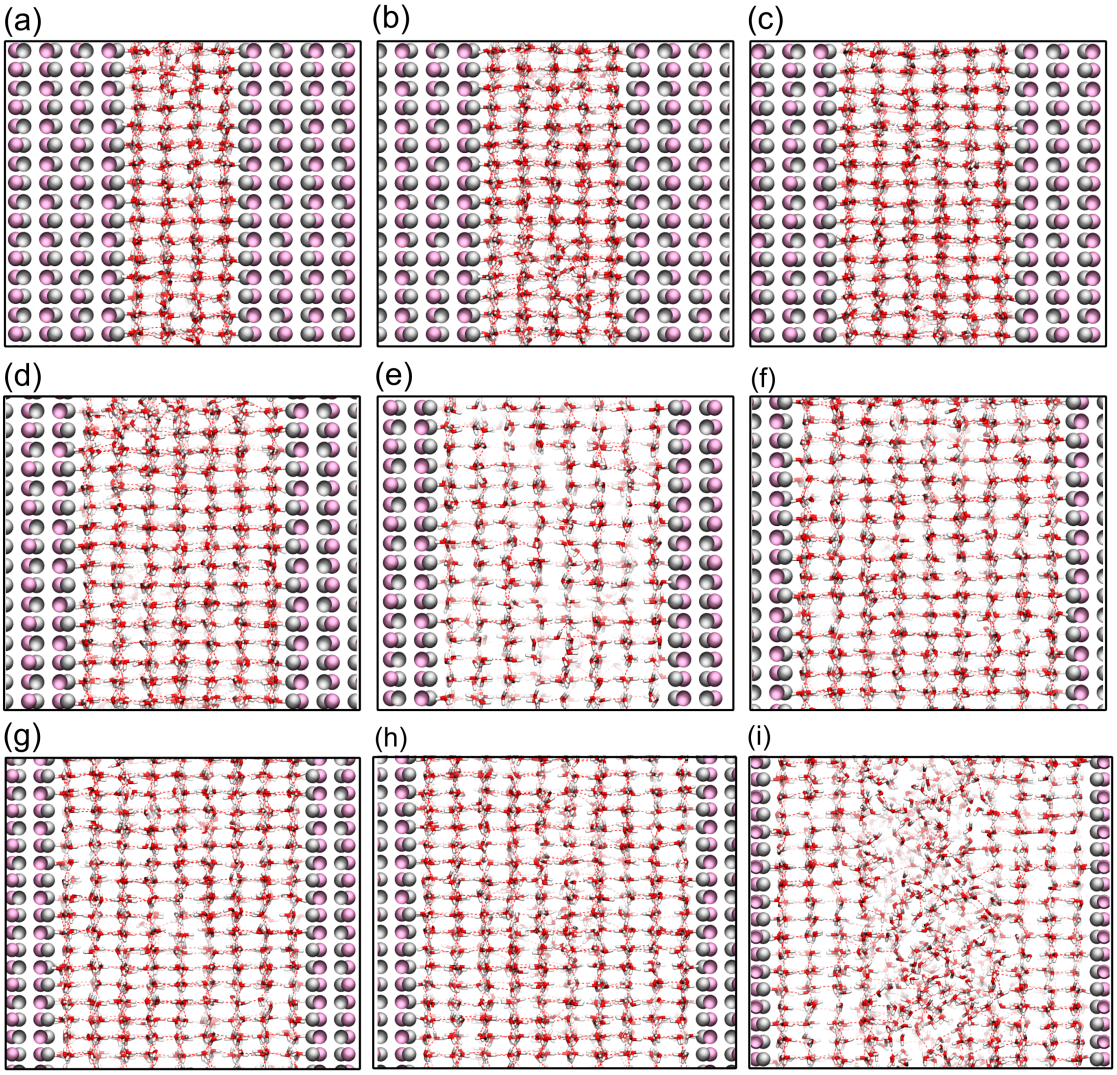

Figure S2. Snapshot details of the last frame of TIP4P/Ice simulations at 265 K for AgI slit systems with gap widths of (a) 4 ice bilayers, (b) 5 ice bilayers, (c) 6 ice bilayers, (d) 7 ice bilayers, (e) 8 ice bilayers, (f) 9 ice bilayers, (g) 10 ice bilayers, (h) 11 ice bilayers and (i) 12 ice bilayers. Ag and I are shown in silver and pink, respectively, and water molecules are shown as red and white sticks.

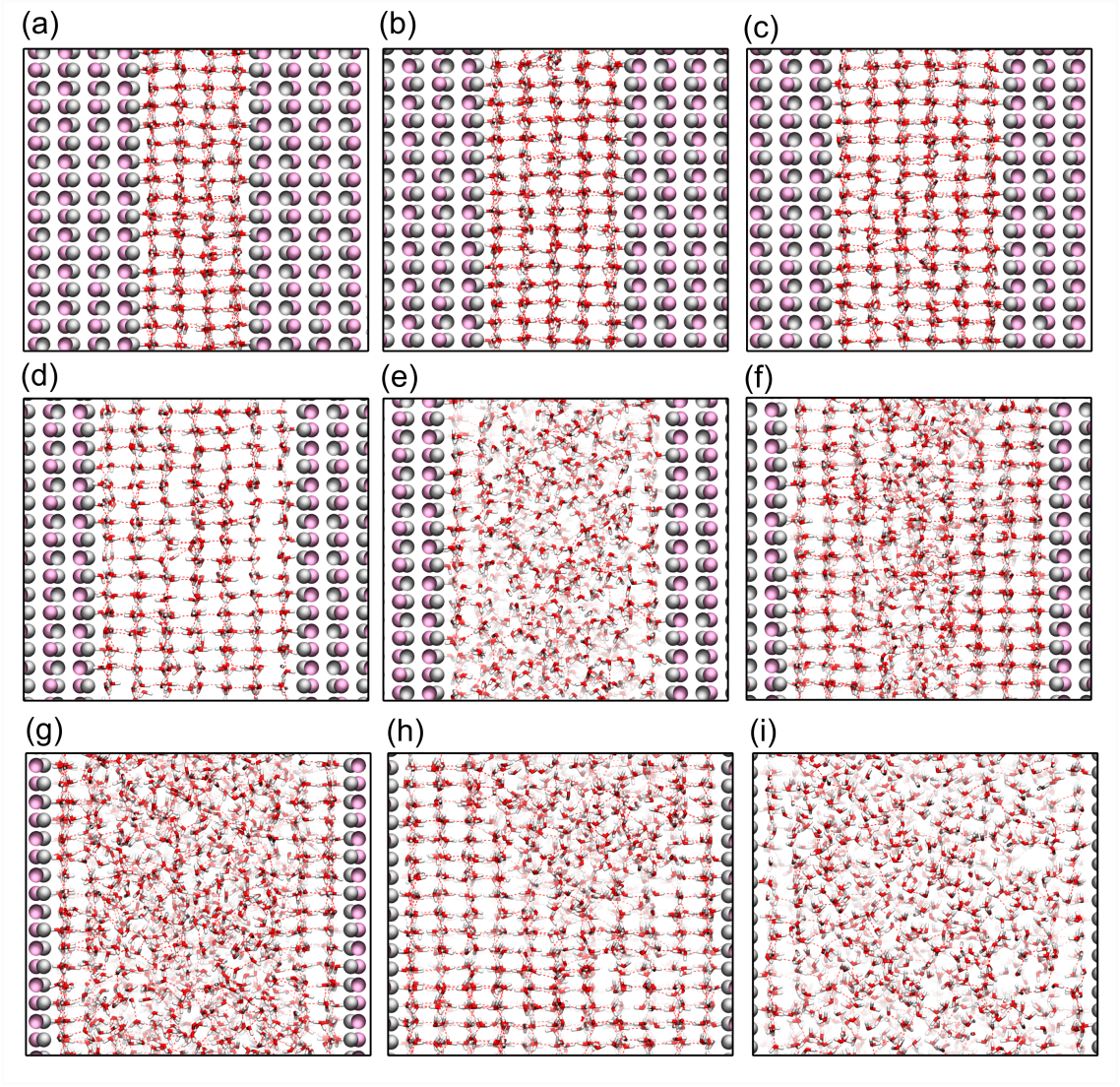

Figure S3. Snapshot details of the last frame of TIP4P/Ice simulations at 267 K for AgI slit systems with gap widths of (a) 4 ice bilayers, (b) 5 ice bilayers, (c) 6 ice bilayers, (d) 7 ice bilayers, (e) 8 ice bilayers, (f) 9 ice bilayers, (g) 10 ice bilayers, (h) 11 ice bilayers and (i) 12 ice bilayers. Ag and I are shown in silver and pink, respectively, and water molecules are shown as red and white sticks.

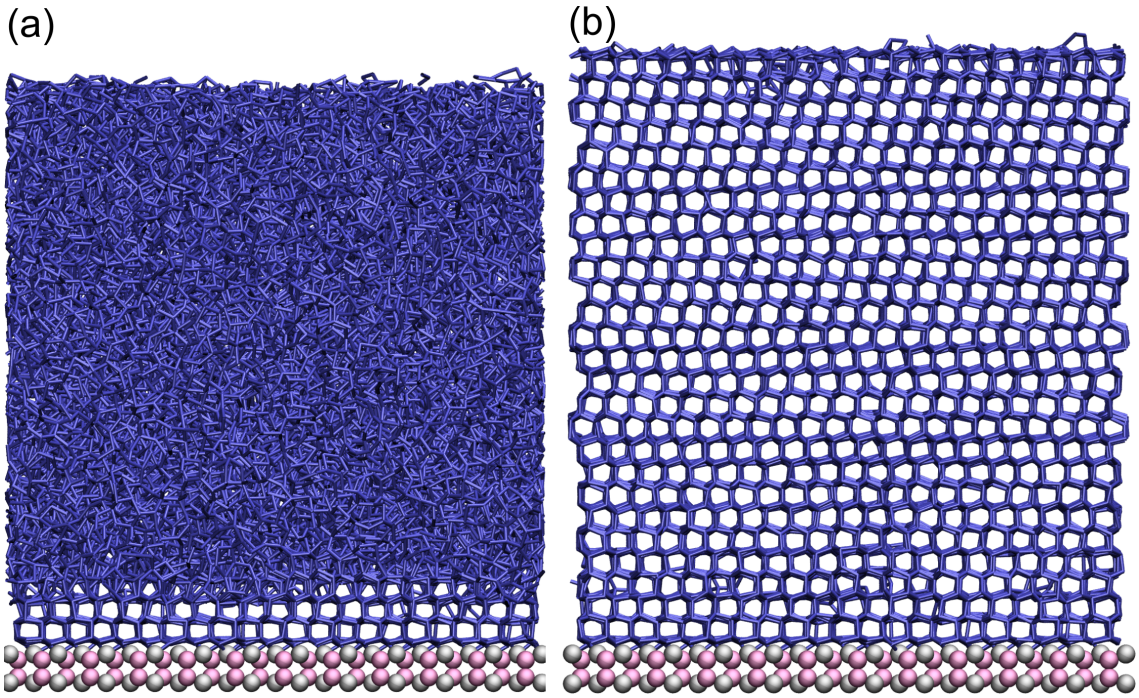

Figure S4. Simulation snapshot details of maximum ice growth observed in ice nucleation simulations on the flat AgI(0001) surface using the mW model (a) at $T = 263$ K in 60 ns, and (b) at 262 K in 20 ns. Ag and I are colored in silver and pink, respectively, and the hydrogen bond network between mW water molecules is indicated by blue sticks.

Table S1. Number of water molecules and simulation box dimensions used in ice nucleation simulations on wedge systems using the TIP4P/Ice water model

Systems	Number of water molecules	box size nm^3
W^{30}	8883	$9.45 \times 7.33 \times 25$
W^{45}	17440	$14.51 \times 7.33 \times 25$
W^{60}	19840	$23.95 \times 7.33 \times 25$
W^{70}	8338	$9.87 \times 7.33 \times 20$
W^{73}	8342	$10.50 \times 7.33 \times 20$
W^{110}	8068	$11.87 \times 7.33 \times 20$
W^{120}	7957	$12.35 \times 7.33 \times 20$

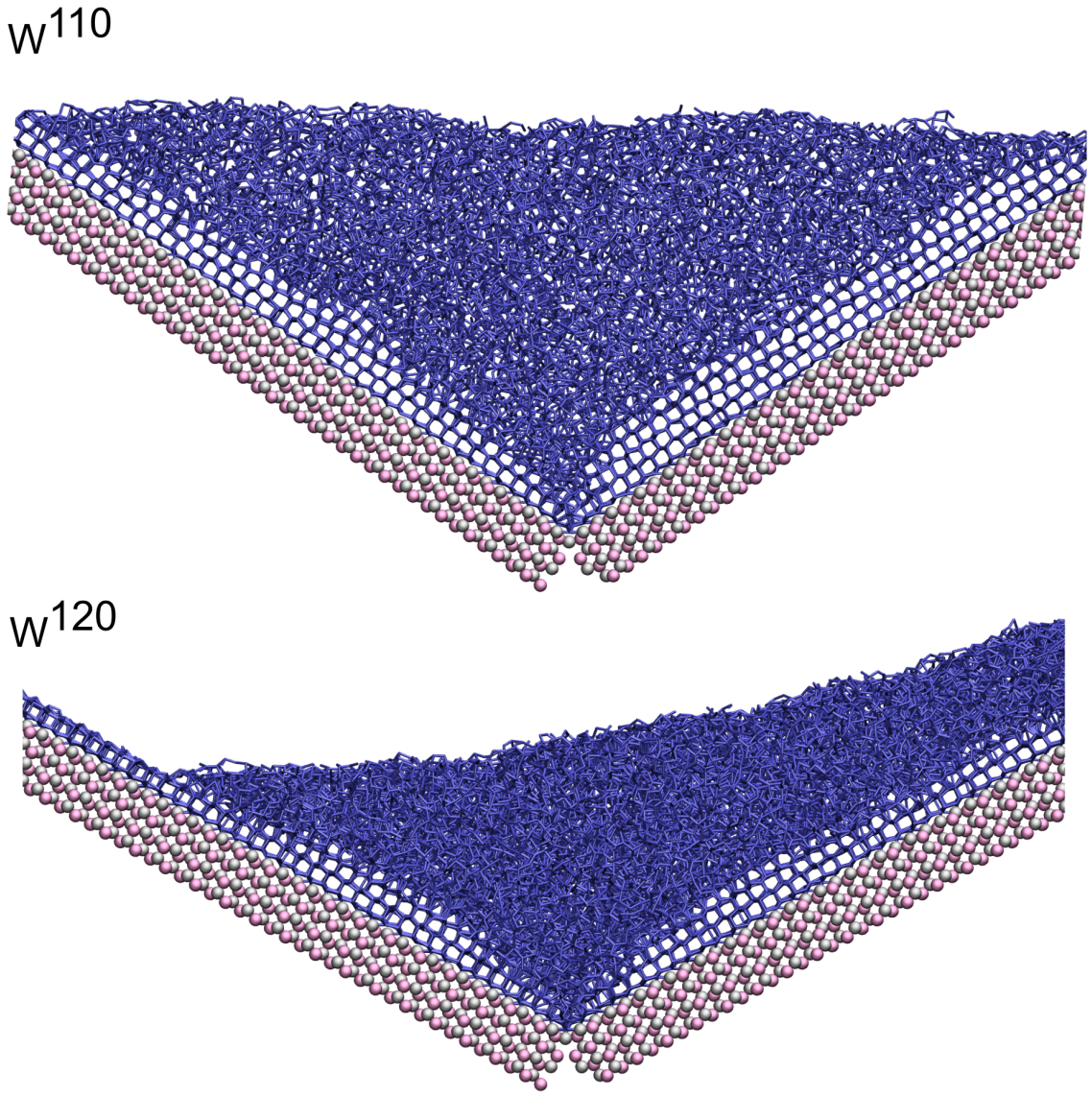

Figure S5. Simulation snapshot details of the last frame ($t = 150$ ns) for wedge systems W^{110} (top) and W^{120} (bottom) at $T = 263$ K, using the mW model. Ag and I are colored in silver and pink, respectively, and the hydrogen bond network between mW water molecules is indicated by blue sticks.

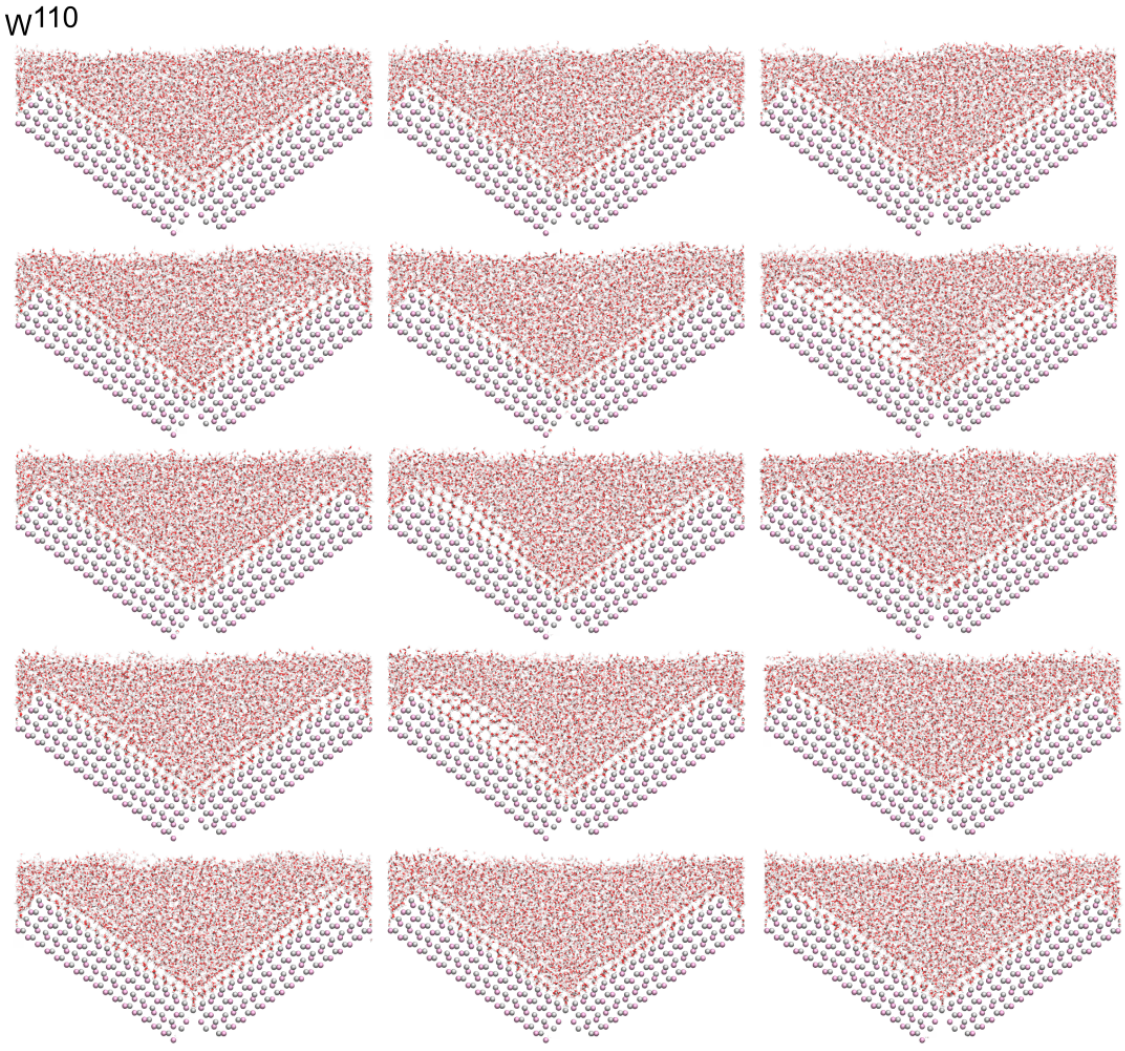

Figure S6. Simulation snapshot details of the last frames of 15 independent simulations of wedge systems W^{110} at $T = 263$ K using the TIP4P/Ice model. Ag and I are shown in silver and pink, respectively, and water molecules are shown as red and white sticks.

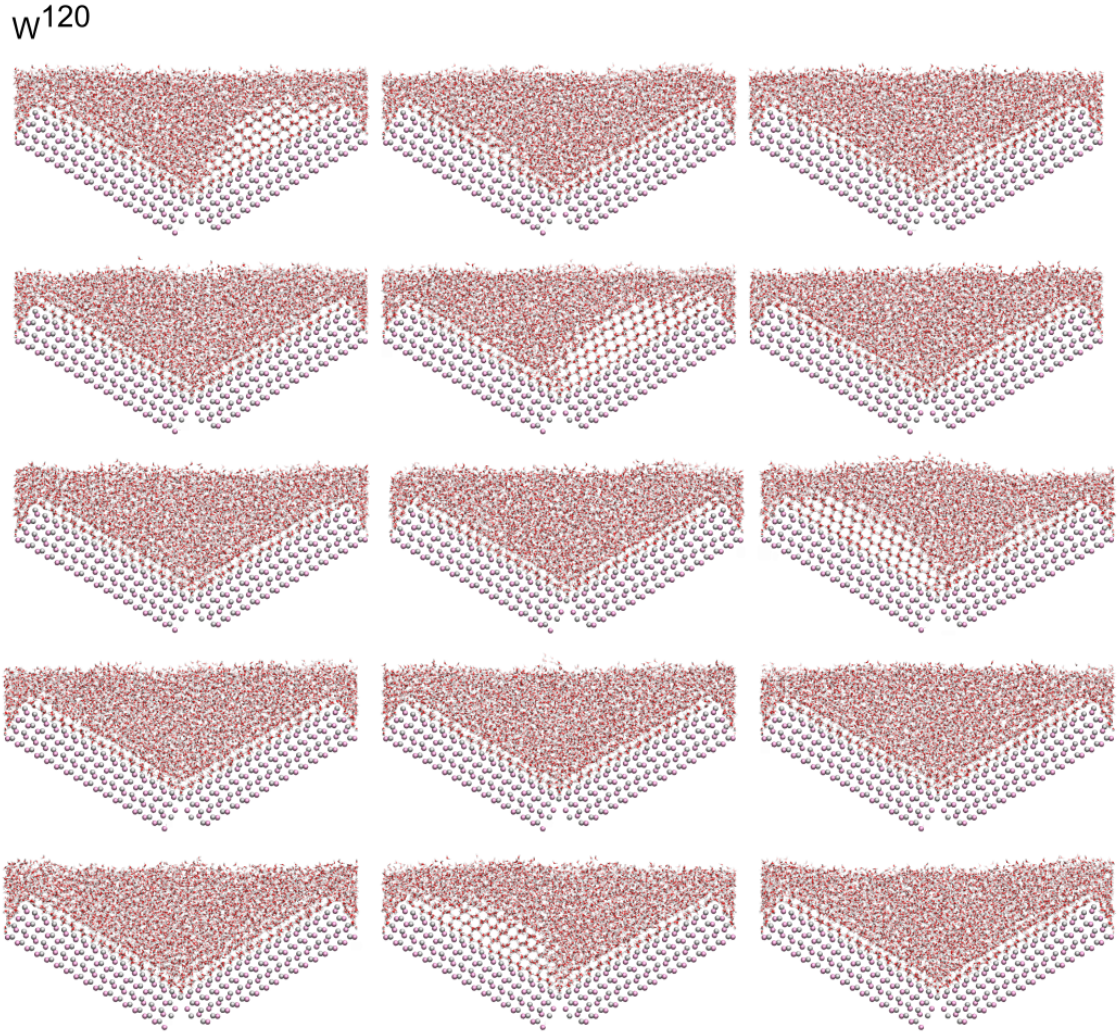

Figure S7. Simulation snapshot details of the last frames of 15 independent simulations of wedge systems W^{120} at $T = 263$ K using the TIP4P/Ice model. Ag and I are shown in silver and pink, respectively, and water molecules are shown as red and white sticks.

Table S2. Number of water molecules and simulation box dimensions used in ice nucleation simulations on wedge systems using the mW water model

Systems	Number of water molecules	box size nm^3
W^{30}	17766	$9.54 \times 7.33 \times 18$
W^{32}	63661	$17.99 \times 10.08 \times 29$
W^{45}	17440	$14.54 \times 7.33 \times 15.4$
W^{60}	30775	$24 \times 7.33 \times 17$
W^{62}	63280	$22.48 \times 10.08 \times 16.1$
W^{70}	18056	$19.1 \times 7.33 \times 15$
$W^{70}_{outgrowing}$	72236	$19.1 \times 7.33 \times 33.5$
W^{73}	19205	$19.5 \times 7.33 \times 15$
$W^{73}_{outgrowing}$	77784	$22.97 \times 7.33 \times 27$
W^{110}	33009	$31.4 \times 7.33 \times 15$
W^{120}	22824	$30.1 \times 7.33 \times 13$

Table S3. Induction times for ice nucleation (ns) for 15 independent simulations of different AgI wedge systems at temperatures 263 K, 265 K and 267 K using the TIP4P/Ice water model. Dashes (-) indicate *no nucleation* event within 150 ns.

Systems	T (K)	Simulations														
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
W^{30}	263	15	63	22	24	5	8	14	25	26	21	4	2	63	66	4
	265	95	50	122	-	-	116	132	12	54	119	18	85	93	30	-
	267	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
W^{45}	263	74	5	34	59	99	61	49	3	83	61	9	62	59	22	47
	265	-	-	-	-	-	-	-	-	-	-	110	-	-	-	-
	267	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
W^{60}	263	2	3	7	2	2	4	4	3	3	3	9	19	3	2	5
	265	12	10	6	23	3	26	4	9	8	6	8	12	9	7	3
	267	11	5	2	5	9	4	3	3	4	2	5	3	6	27	7
W^{70}	263	-	121	-	-	-	82	86	-	11	-	-	9	-	-	87
	265	-	-	78	-	-	-	-	-	-	-	-	-	-	-	-
	267	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
W^{73}	263	10	28	10	32	8	5	18	51	45	9	86	28	11	18	40
	265	20	43	7	-	17	3	59	-	-	74	61	37	15	13	119
	267	-	-	129	-	-	-	133	-	-	-	-	-	-	-	-
W^{110}	263	-	-	-	-	17	120	-	-	-	-	-	134	-	-	129
	265	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	267	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
W^{120}	263	-	-	66	-	-	7	-	-	-	44	-	-	-	-	-
	265	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	267	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table S4. Fraction of simulations exhibiting an ice nucleation event for different AgI wedge systems at temperatures 265 K and 267 K using the mW water model.

Systems	T (K)	Number of nucleation events
W^{30}	265	15/15
	267	0/15
W^{32}	265	15/15
	267	0/15
W^{62}	265	15/15
	267	0/15
W^{70}	265	15/15
	267	15/15
W^{73}	265	12/15
	267	0/15