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Electronic Supplementary Information

The effect of solvents on morphology of sulfamerazine crystals and its molecular mechanism

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Table S1. Crystal habit relevant parameters of SMR in different solvents calculated by the MAE model.

Solvent	Faces	E_{tot}	E_{sol}	E_{sur}	E_{int}	E_s	Eatt'	R'_{hkl}	Area/%
Water	001	-1950.03	-2687.92	15276.45	-70.92	-81.46	24.15	1.80	32.35
	011	-1464.03	-2210.50	30769.23	-146.45	-220.12	133.75	9.95	--
	100	-1763.75	-2979.97	15297.41	-68.69	-67.11	-13.44	1.00	58.52
	110	-1470.35	-2181.99	30706.93	-146.32	-200.20	105.99	7.89	--
	201	-1445.88	-2176.76	30666.00	-146.02	-163.67	79.83	5.94	--
	111	-1221.46	-2130.96	30675.46	-145.20	-194.48	96.20	7.16	9.13
Methanol	001	45.78	-1228.19	15276.46	-68.30	-78.46	21.14	1.50	36.25
	011	629.10	-647.39	15297.41	-143.87	-216.23	129.86	6.14	--
	100	326.67	-1028.10	30769.23	-68.01	-66.45	-14.10	1.00	54.32
	110	612.86	-626.89	30706.93	-143.74	-196.68	102.47	7.27	--
	201	649.37	-645.23	30666.00	-143.28	-160.58	76.75	5.44	--
	111	1024.75	-655.74	30675.47	141.44	-189.44	91.16	6.47	9.43
Ethanol	001	-2707.99	-4610.44	15276.46	-65.24	-74.94	17.62	1.08	43.56
	011	-2097.15	-3910.46	30769.23	-141.25	-212.30	125.93	7.73	--
	100	-2500.78	-4316.22	15297.41	-65.77	-64.26	-16.30	1.00	46.43
	110	-1813.32	-3983.89	30706.93	-139.20	-190.46	96.25	5.90	--
	201	-2068.39	-3867.28	30666.00	-140.82	-157.83	73.99	4.54	--
	111	-1395.66	-3869.23	30675.47	-137.58	-184.26	85.98	5.27	10.01
Isopropanol	001	-6242.42	-8673.56	15276.46	-62.66	-71.97	14.66	1.00	51.23
	011	-5425.10	-7813.81	30769.23	-138.44	-208.08	121.71	8.30	--
	100	-5895.27	-8284.95	15297.41	-62.96	-61.52	-19.04	1.30	38.24
	110	-5417.72	-7762.15	30706.93	-138.36	-189.30	95.09	6.49	--
	201	-5392.89	-7751.80	30666.00	-138.08	-154.77	70.93	4.84	--
	111	-4389.31	-7722.84	30675.47	-133.38	-178.64	80.36	5.48	10.53
Methyl acetate	001	-1921.47	-4137.82	15276.46	-63.71	-73.18	15.86	1.00	48.29
	011	-1002.13	-3140.23	30769.23	-139.66	-209.92	123.54	7.79	--
	100	-1425.94	-3630.98	15297.41	-63.87	-62.40	-18.16	1.15	41.14
	110	-927.34	-3059.89	30706.93	-139.39	-190.72	96.51	6.09	--
	201	-942.88	-3101.64	30666.00	-139.06	-155.86	72.03	4.54	--
	111	88.98	-3052.34	30675.47	-134.31	-179.80	81.62	5.15	10.57
Ethyl acetate	001	-3366.44	-6139.06	15276.46	-60.99	-70.06	12.74	1.00	56.29
	011	-2819.01	-5537.94	30769.23	-136.83	-205.66	119.29	9.36	--
	100	-3516.80	-6263.74	15297.41	-61.22	-59.82	-20.74	1.63	33.12
	110	-2769.81	-5476.85	30706.93	-136.58	-186.88	92.67	7.27	--
	201	-2718.63	-5405.42	30666.00	-136.48	-152.97	69.14	5.43	--
	111	-1474.66	-5394.36	30675.47	-130.52	-174.81	76.53	6.01	10.59
Butyl acetate	001	7231.33	3811.20	15276.46	-57.84	-66.43	9.12	1.00	67.63
	011	-2617.52	-6457.13	30769.23	-131.36	-197.44	111.07	12.18	--
	100	-3218.05	-7115.37	15297.41	-55.61	-54.33	-26.22	2.88	21.57
	110	-2532.20	-6320.33	30706.93	-131.31	-179.67	85.46	9.37	--

	201	-2470.33	-6296.31	30666.00	-130.93	-146.74	62.91	6.90	--
	111	-706.64	-6231.03	30675.47	-122.69	-164.33	66.05	7.24	10.80

All energies are in kcal·mol^{-1}.

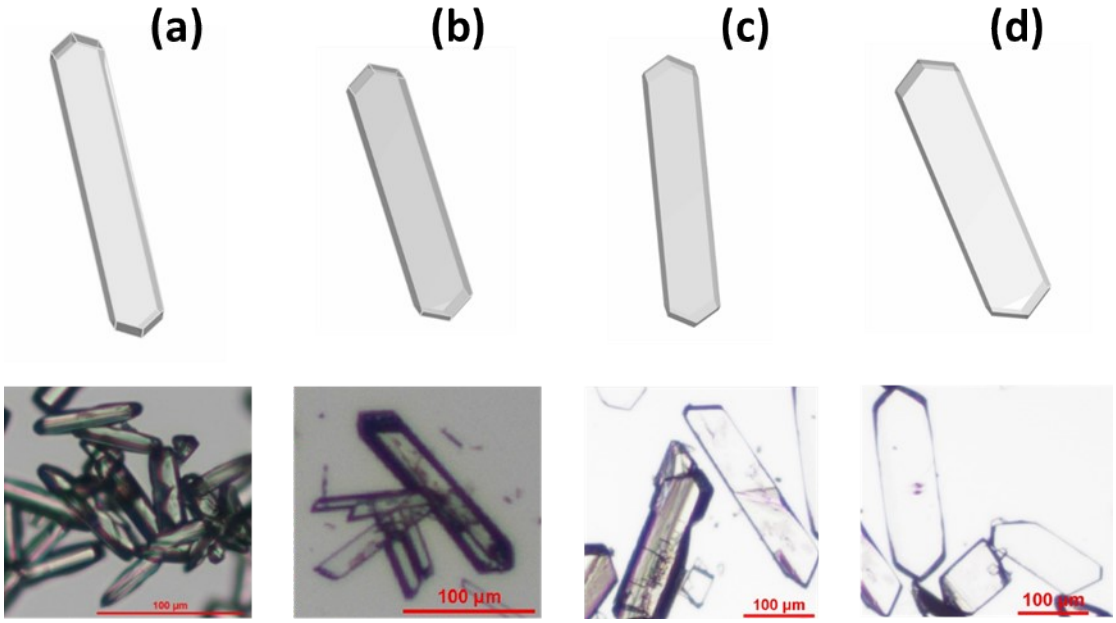

Fig S1. The modified morphology predicted in ethanol (a), isopropanol (b), methyl acetate (c) and ethyl acetate (d) with MAE model.

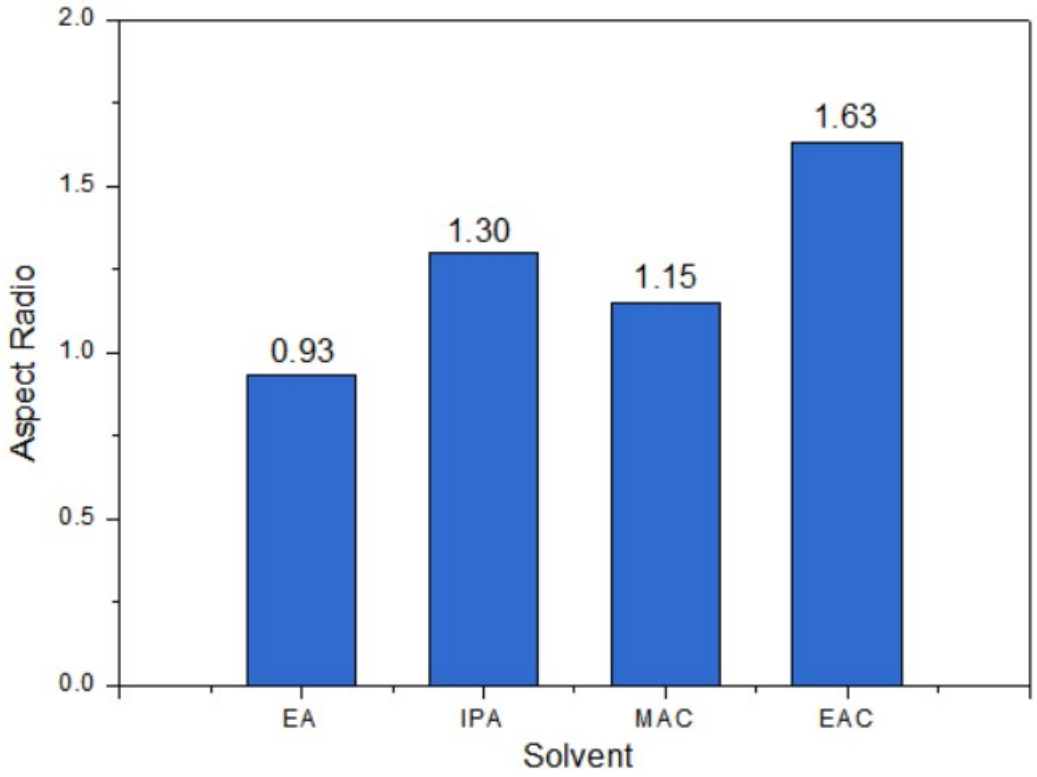

Fig S2. The simulated aspect ratios of SMR crystals in ethanol, isopropanol, methyl acetate and ethyl acetate.

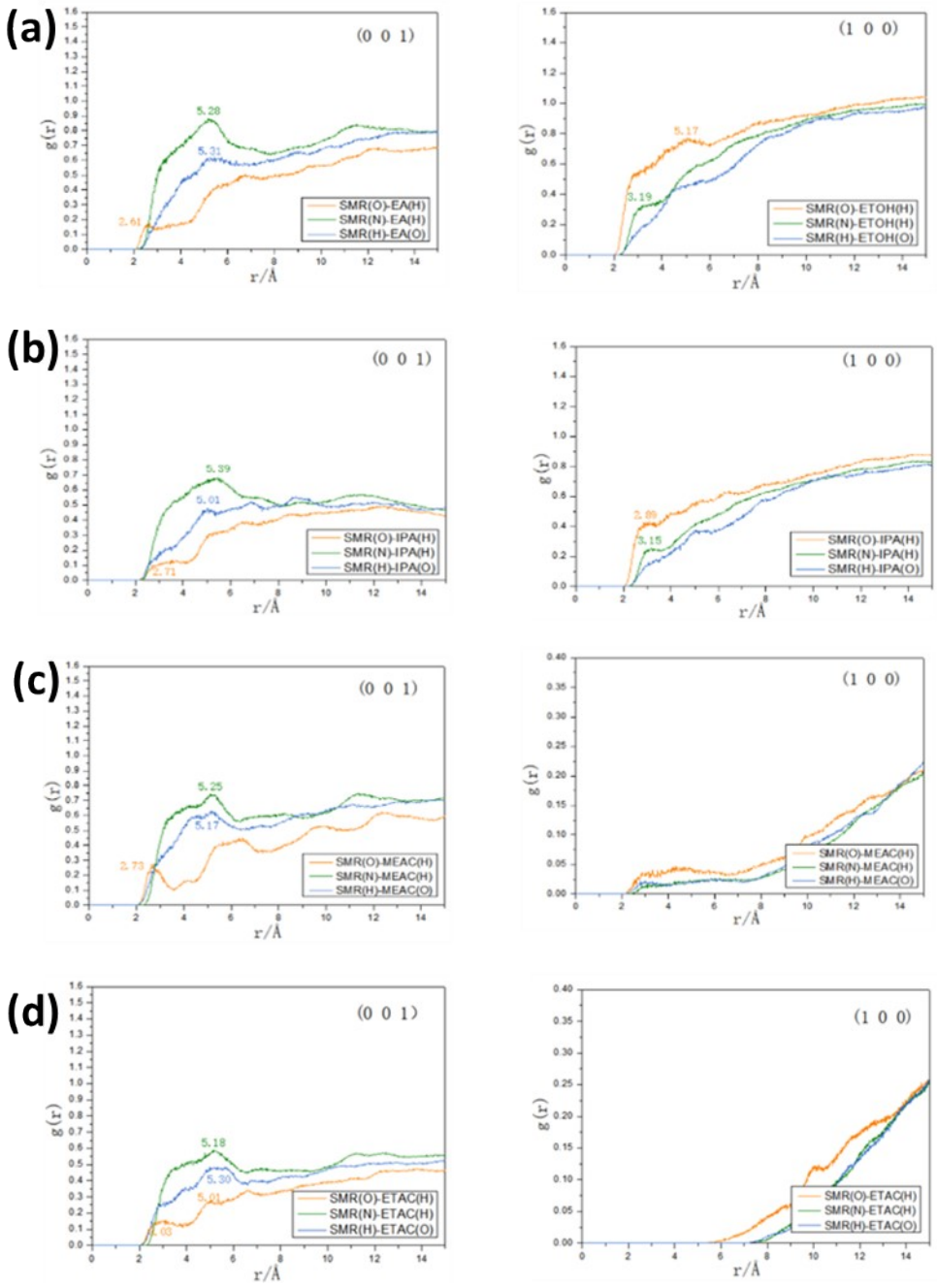

Fig S3. The RDF curves of (a)ethanol, (b)isopropanol, (c) methyl acetate and (d)ethyl acetate with (0 0 1) (left) and (1 0 0) (right) faces. Black, red, and blue lines represent the interactions of SMR(O)-solvent (H), SMR (N)-solvent (H), and solute (H)-solvent (O), respectively.

Model size convergence

The model dimension can dramatically influence E_s, which significantly affects the final predicted morphology. And it is well known that the lager the model dimension, the more accurate the result will be. This is because for the non-bonding interactions, the molecules in the model may be affected by the mirror self-molecules in the mirror periodic box. But if the model dimension is too large, the simulation time will inevitably increase, and the accuracy will not increase significantly. Therefore, it is a crucial step to find an appropriate model dimension to meet the accuracy and to consume less time. In this study, the model size was validated by the controlled variable method, and the effects of crystal surface layer thickness (t_c), solvent layer thickness (t_s) or the number of solvent molecules, vacuum layer thickness (t_v) and the length (U) and width (V) of the supercell on E_s were investigated one by one. Additionally, when constructing the amorphous cell of the solvent, the NVT ensemble was first used for the production of the solvent phase with 500 ps simulation time, and then the NPT ensemble was applied for the equilibration of the solvent phase with 500 ps. Taking the (0 0 1) surface of SMR as an example, the procedures are summarized in Fig. S4, and the calculated E_s values affected by the model dimension are summarized in Table S4 and Fig. S5~S11.

The simulation results illustrate that with the increase in t_c, t_s, t_v, U and V, the E_s values decrease (or increase) rapidly initially and then remain almost constant.

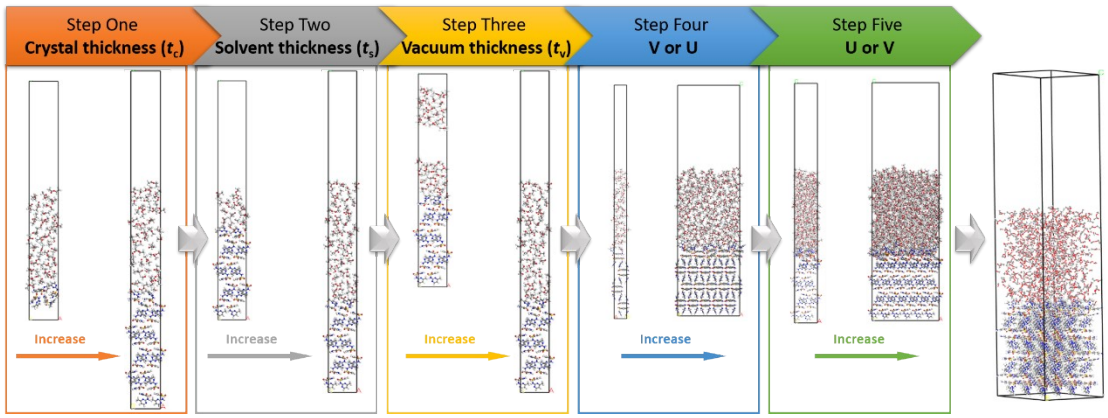

Fig. S4 The investigation procedure of the effect of model dimension on the E_s.

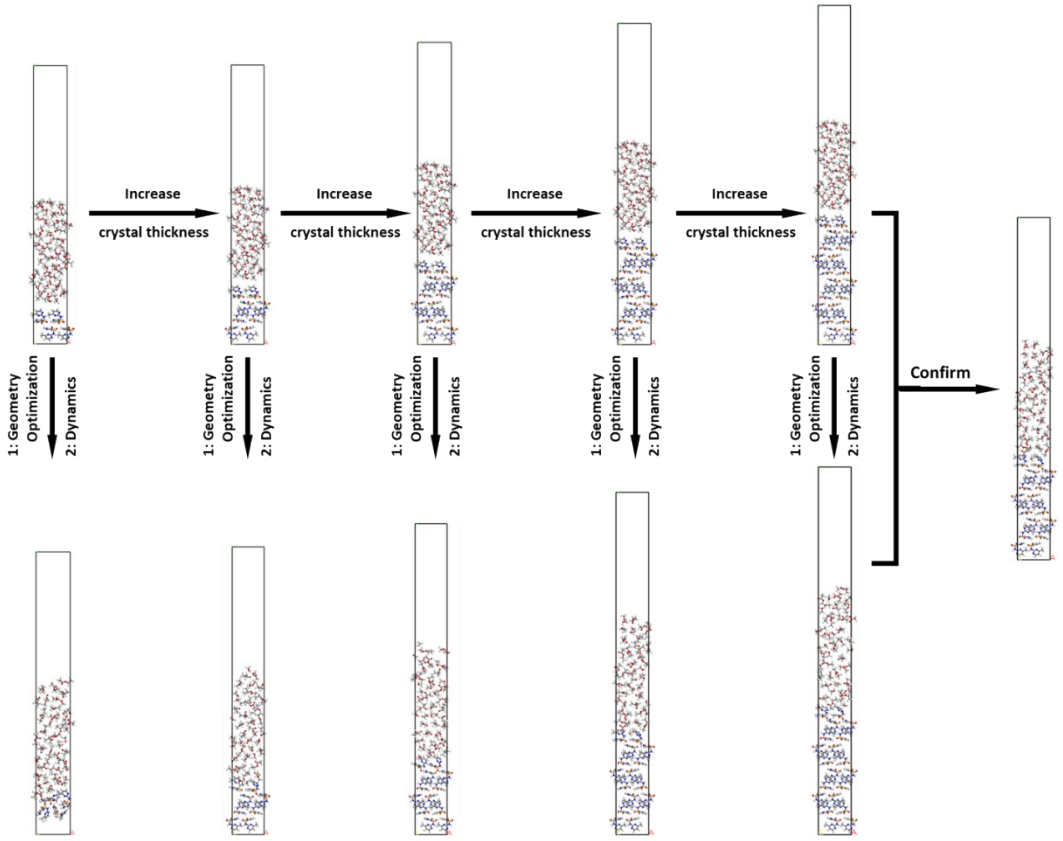

Fig. S5 Details of confirming the crystal thickness.

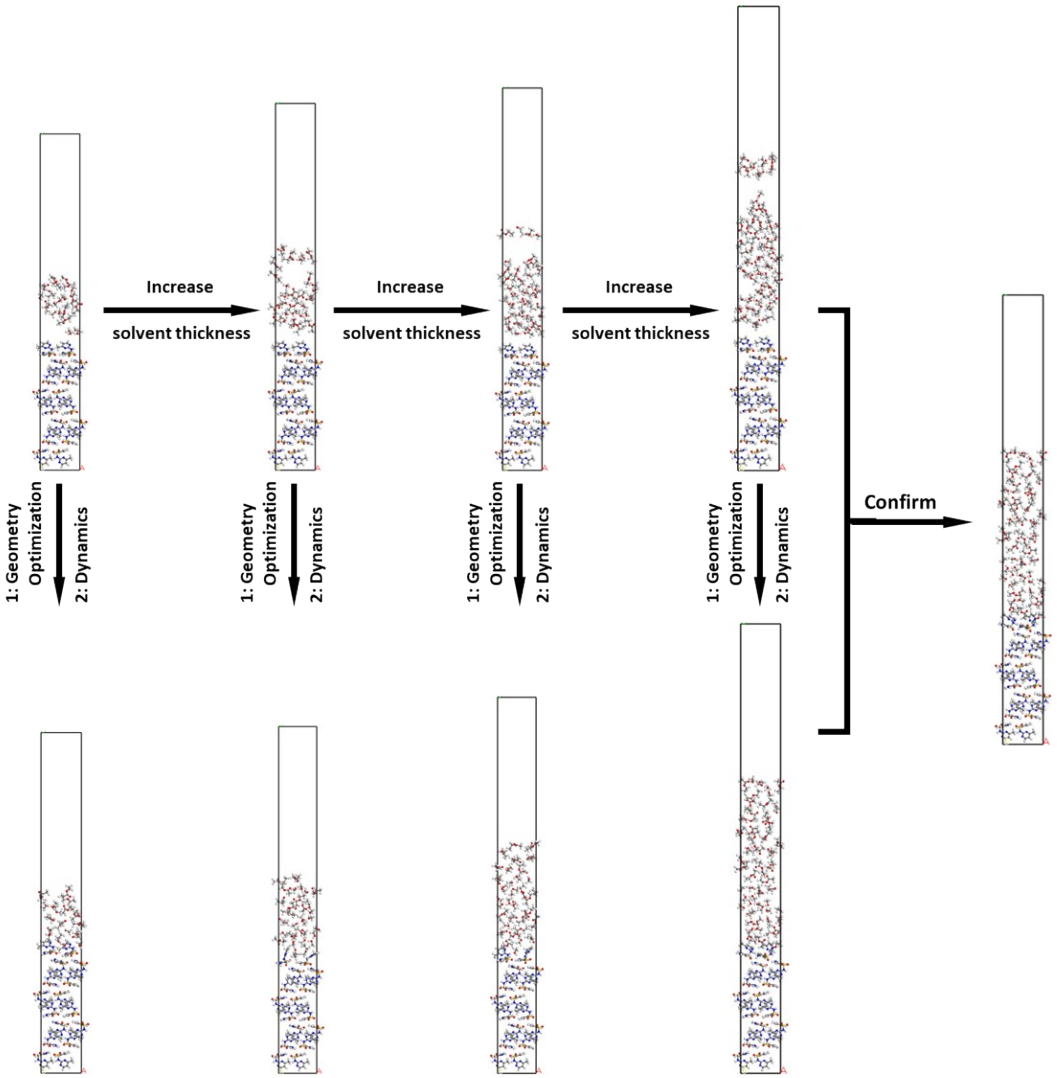

Fig. S6 Details of confirming the solvent thickness or the number of solvent molecules.

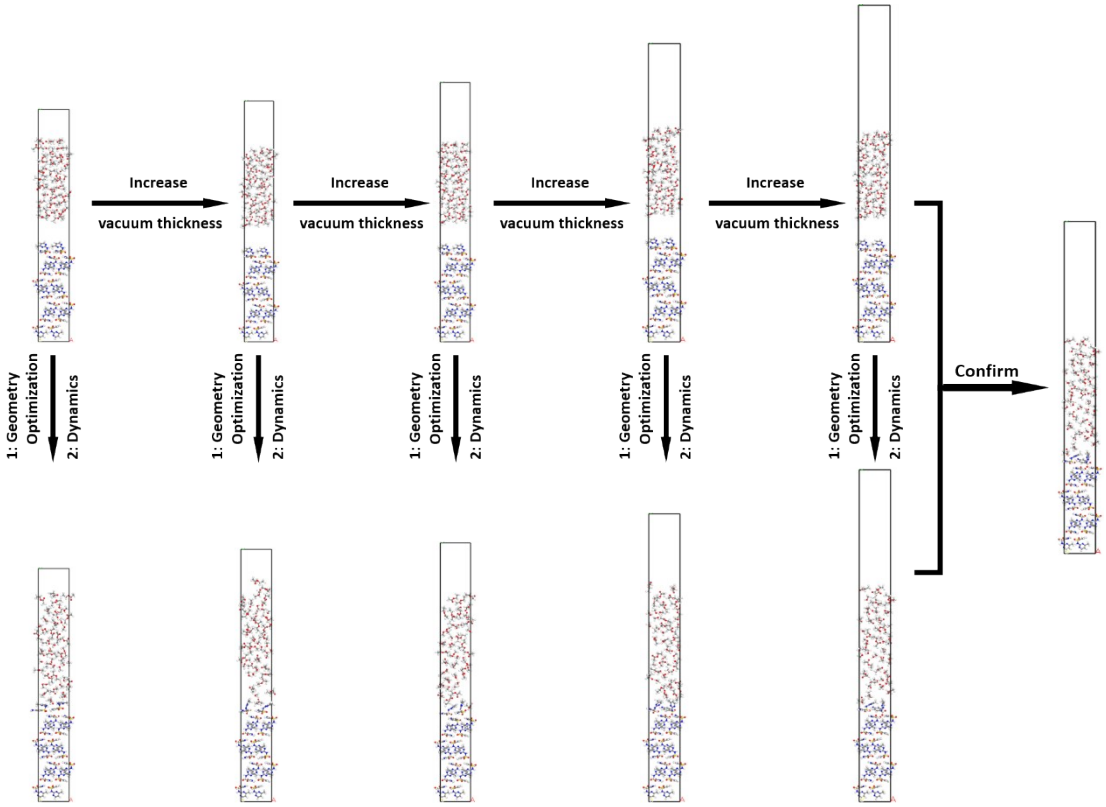

Fig. S7 Details of confirming the vacuum thickness.

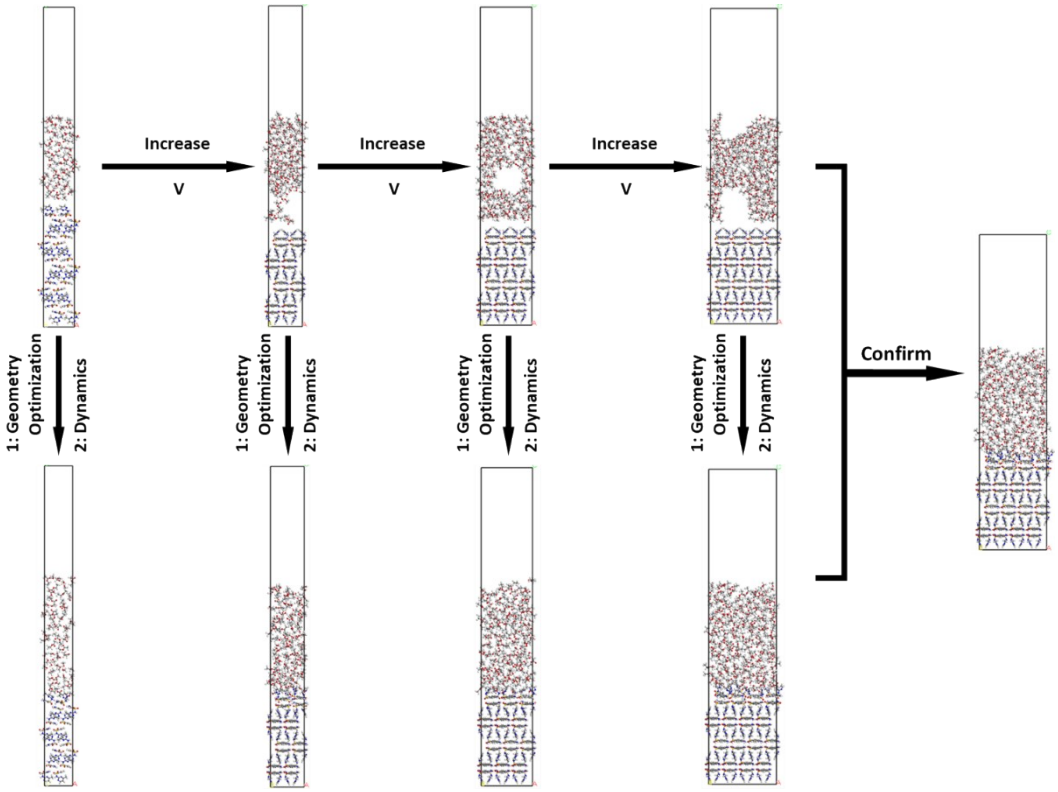

Fig. S8 Details of confirming the V.

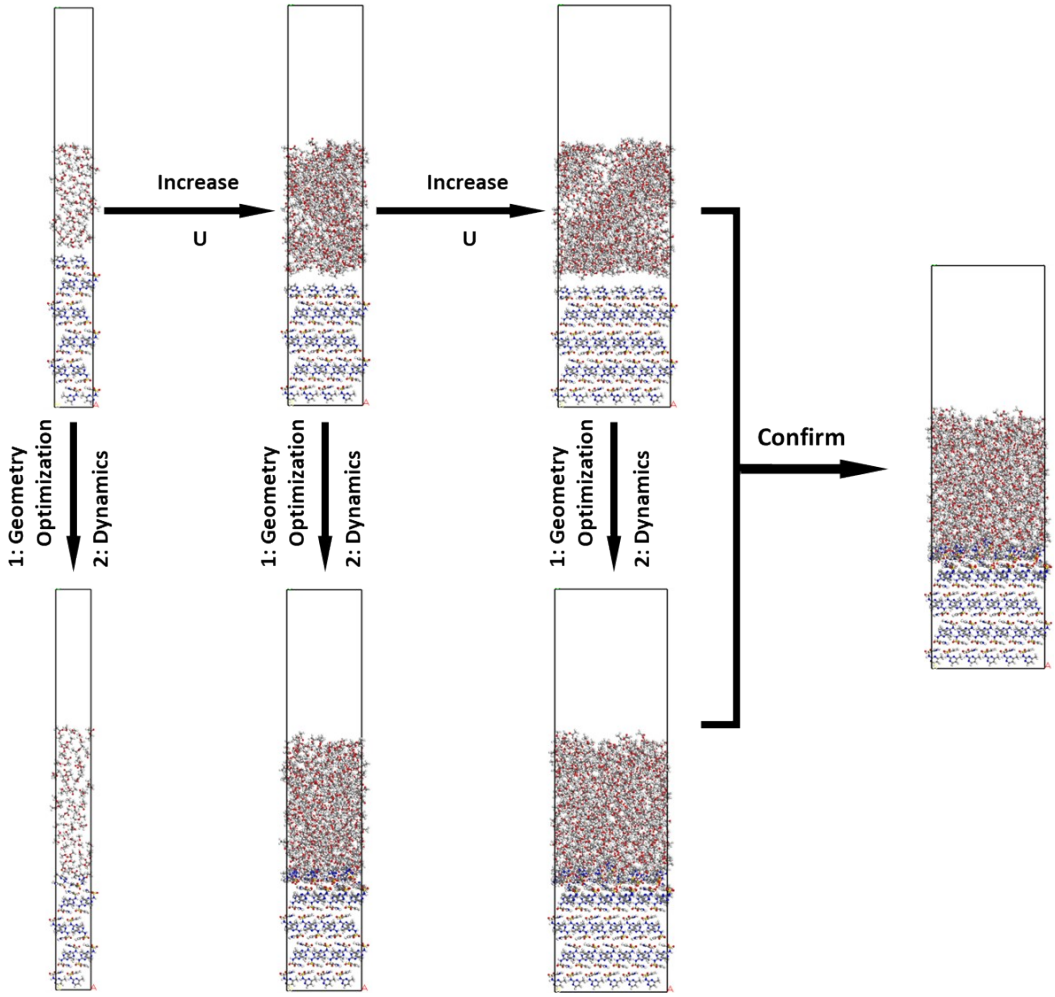

Fig. S9 Details of confirming the U.

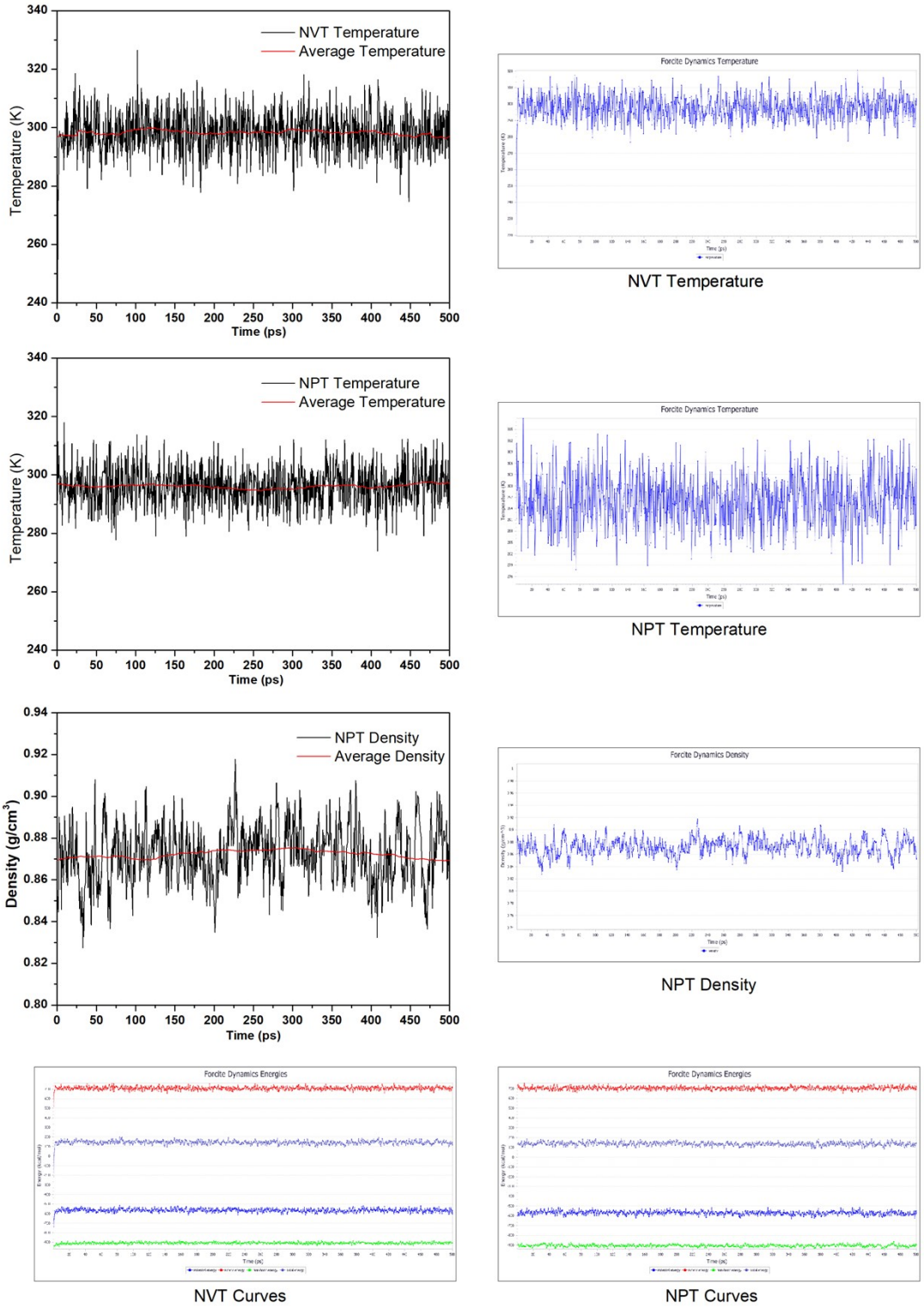

Fig. S10 The fluctuation curves of energy, temperature and density of amorphous cell and the crystal-solvent interface model preforming on NPT and NVT ensemble, respectively.

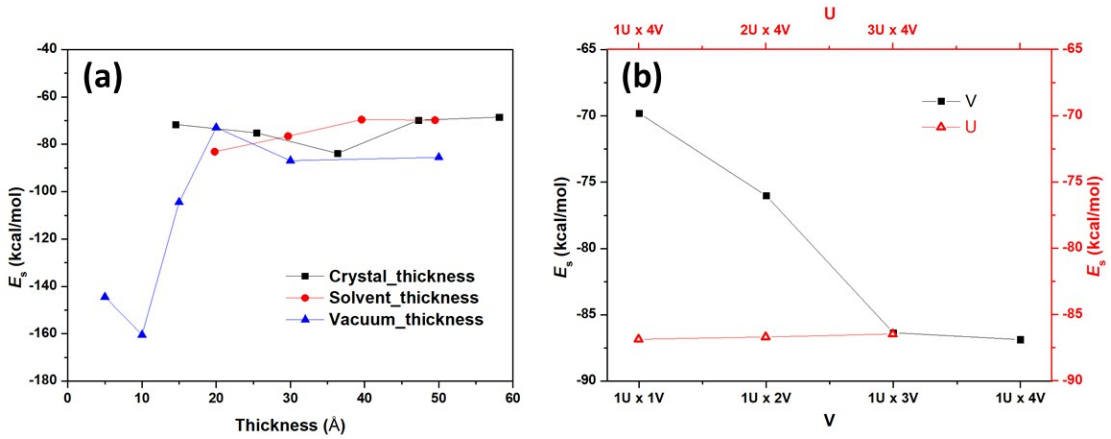

Fig. S11 The influence of model dimension on E_s.

Table S2 The determination of the model dimensions

face	Thickness										U	V
	Crystal	Solvent (Number of the solvent molecules)								Vacuum		
	Mix & Pure	Mix	H2O	MeOH	EtOH	IPA	MeAc	EtAc	BuAc	Mix & Pure	Mix & Pure	Mix & Pure
(001)	4t (47.2508Å)	600	1320	960	600	600	480	360	360	50Å	3U (43.4319Å)	4V (32.7480Å)
(011)	4t (36.5263Å)	1200	4800	2400	1440	1440	1080	960	600	50Å	4U (57.9092Å)	3V (69.8531Å)
(100)	4t (33.7756Å)	750	3000	1500	1050	1050	750	600	450	50Å	5U (40.9350Å)	3V (65.3928Å)
(110)	4t (34.4933Å)	660	2400	1200	780	780	600	480	360	50Å	2U (43.5929Å)	3V (49.8956Å)
(201)	4t (31.1143Å)	600	2400	1200	780	780	600	480	360	50Å	1U (45.9362Å)	6V (49.1220Å)
(111)	5t (39.0131Å)	1560	5400	2400	1800	1800	1320	960	720	50Å	4U (66.5275Å)	3V (69.8531Å)