Experiments:

In experiments, microscopy and PIV (Particle Image Velocimetry) techniques were used to observe the evolution of the solid-liquid interface and flow field of the droplet during the droplet spreading on glucose surface. The experimental process includes: (1) Preparing a soluble solid substrate. Firstly, making a mold with PDMS (Polydimethylsiloxane), and then pouring the molten glucose into the mold, when it cools to room temperature, a solid substrate is obtained after it was decoated from the mold. (2) Preparing droplet containing tracer particles, and then the internal flow field of the droplet can be observed by PIV technology. During the preparation process, it is important that tracer particles with a small particle size (6 μm) should be selected, and after it is added to the water, it is also necessary to use an ultrasonic cleaning instrument for shaking so that the particles are evenly distributed in water. Once a solid substrate is obtained, the experiments were carried out in an ultra-clean environment. The lens was adjusted to the side of the specimen, a micro syringe was used to generate droplets with a diameter of 0.5 mm and release the droplet on the solute surface. The relevant experimental data were recorded and extracted by a high-speed camera.

Input parameters settings for machine learning:

(1) solid-solid interactions:

As shown in figure 4, by all-atomic simulations, we obtained a glucose system in equilibrium. At this point, an approximate $\sigma_{s\text{-}s}$ (6.0 Å) can be obtained by averaging the distance between glucose molecules, as shown in figure S1 (a).

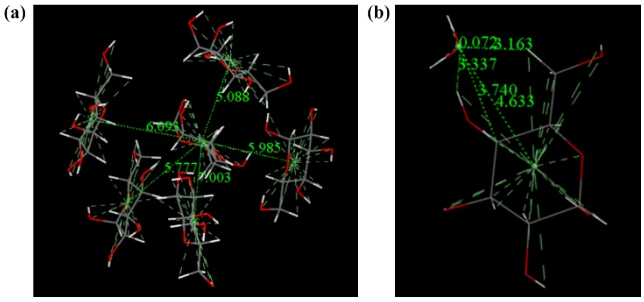

Figure S1. (a) Centroid spacing of glucose molecules in equilibrium. (b) The distance between water molecule and every glucose atom

For simplicity, the initial value of $\varepsilon_{s\text{-}s}$ is obtained by all-atomic interactions between water and glucose molecules. Firstly, placing a water molecule near the glucose as shown in figure S1 (b), then calculating the distance between water molecule and every glucose atom. The total interaction can be calculated as follows:

$$E_{glucose-water}=\sum_{i=1}^{24}4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12}-\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] \qquad \text{* MERGEFORMAT (1)}$$

For coarse-grained models, the interaction between water and glucose can be calculated as:

$$E_{CG-water}=4\varepsilon_{CG-water}\left[\left(\frac{\sigma_{CG-water}}{r_{CG-water}}\right)^{12}-\left(\frac{\sigma_{CG-water}}{r_{CG-water}}\right)^{6}\right] \qquad \text{* MERGEFORMAT (2)}$$

in which $\sigma_{CG\text{-}water}$ was calculated by Lorentz-Berthelot rules[42], i.e., $\sigma_{CG\text{-}water}$= (6.0+3.165)/2=4.583 Å, and $r_{CG-water}$ is obtained from Figure S1(b) and equals to 4.633 Å. It is reasonable to assume that the value of the Eq. (1) is equal to the value of the Eq. (2), and as shown in Table S1, the $\varepsilon_{CG-water}$ can be obtained. Again, following Lorentz-Berthelot rules[42], an approximate $\varepsilon_{s\text{-}s}$ (3.89 kcal/mol) can also be obtained.

Table S1 The total interaction between water and glucose

all-atomic		ε	σ		εs-l	σs-l			rij	Eij
pair_coeff	CA	0.0528	3.5		0.091913	3.335	Glucose-Water	C-H2O	3.458	-0.069217549
pair_coeff	CD	0.0528	3.5		0.091913	3.335		C-H2O	3.74	-0.091429971
pair_coeff	CE	0.0528	3.5		0.091913	3.335		C-H2O	4.977	-0.029523001
pair_coeff	CG	0.0528	3.5		0.091913	3.335		C-H2O	5.543	-0.017365782
pair_coeff	H	0.024	2.5		0.0619677	2.835		C-H2O	4.194	-0.069055309
pair_coeff	HA	0	0		0	1.585		C-H2O	5.916	-0.011601061
pair_coeff	HD	0	0		0	1.585		H-H2O	2.776	0.020665331
pair_coeff	HE	0.024	2.5		0.0619677	2.835		H-H2O	3.163	-0.061900451
pair_coeff	HG	0.024	2.5		0.0619677	2.835		H-H2O	2.823	0.020665331
pair_coeff	Hw	0	0	SPC/Fw(Wu 2006)				H-H2O	5.85	-0.003013375
pair_coeff	OA	0.136	3.12		0.1475127	3.145		H-H2O	5.004	-0.007962478
pair_coeff	OD	0.136	3.07		0.1475127	3.12		H-H2O	5.138	0
pair_coeff	OE	0.112	2.9		0.1338656	3.035		H-H2O	3.337	0
pair_coeff	Ow	0.155425	3.165492	SPC/Fw(Wu 2006)				H-H2O	4.644	0
								H-H2O	7.2	0
								H-H2O	6.432	0
								H-H2O	5.085	-0.007097676
								H-H2O	6.569	-0.001547191
								O-H2O	4.636	-0.054109949
								O-H2O	6.84	-0.005453717
								O-H2O	6.839	-0.005453717
								O-H2O	5.033	-0.032777103
								O-H2O	4.025	-0.102954869
								O-H2O	4.911	-0.028527448
							Etotal			-0.557659983
							εs-s			3.888275507

Based on rough initial parameters, the relevant 24×26 potential function parameters ($\sigma_{s\text{-}s}$: from 4.7 Å to 7.0 Å increases by 0.1, $\varepsilon_{s\text{-}s}$: from 3.0 kcal/mol to 5.5 kcal/mol increases by 0.1) are constructed to obtain the corresponding energy and density data sets of the coarse-grained model.

(2) solid-liquid interactions:

$\varepsilon_{s\text{-}l}$ is an important factor that affects the wettability and dissolution rate of solid, thus the inputs values of $\varepsilon_{s\text{-}l}$ in neural networks is determined based on $\varepsilon_{s\text{-}s}$. The detailed values are listed in table S2:

Table S2 The input values of $\varepsilon_{s\text{-}l}$

298 K																								
σss=4.3 kcal/mol ,σss=4.4 kcal/mol,σss=4.5 kcal/mol,σss=4.6 kcal/mol																								
εsl/εss																								
0.3	0.32	0.34	0.36	0.38	0.4	0.42	0.44	0.46	0.48	0.5	0.6	0.7	0.8	0.9	1	1.05	1.1	1.15	1.2	1.25	1.3	1.35	1.4	1.45	1.5
303 K																								
σss=4.3 kcal/mol ,σss=4.4 kcal/mol,σss=4.5 kcal/mol,σss=4.6 kcal/mol																								
εsl/εss																								
0.3	0.32	0.34	0.36	0.38	0.4	0.42	0.44	0.46	0.48	0.5	0.6	0.7	0.8	0.9	1	1.05	1.1	1.15	1.2	1.25	1.3	1.35	1.4	1.45	1.5
308 K																								
σss=4.3 kcal/mol ,σss=4.4 kcal/mol,σss=4.5 kcal/mol,σss=4.6 kcal/mol																								
εsl/εss																								
0.3	0.32	0.34	0.36	0.38	0.4	0.42	0.44	0.46	0.48	0.5	0.6	0.7	0.8	0.9	1	1.05	1.1	1.15	1.2	1.25	1.3	1.35	1.4	1.45	1.5
312 K																								
σss=4.3 kcal/mol ,σss=4.4 kcal/mol,σss=4.5 kcal/mol,σss=4.6 kcal/mol																								
εsl/εss																								
0.3	0.32	0.34	0.36	0.38	0.4	0.42	0.44	0.46	0.48	0.5	0.6	0.7	0.8	0.9	1	1.05	1.1	1.15	1.2	1.25	1.3	1.35	1.4	1.45	1.5