Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Information

Tailoring the phase diagram of discotic mesogens

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ISOTENSION-ISOTHERMAL ENSEMBLE

Monte Carlo simulations in the Isotension-Isothermal ensemble to a system of anisotropic particles requires some minor precautions. The formalism was developed by Parrinello and Rahman [1, 2] and subsequently incorporated to Monte Carlo frameworks by different authors, with the first publication usually attributed to Najafabadi [3]. The aim of this approach is to avoid any artificial stress on the anisotropic particles from the simulation box and the associated boundary conditions. To this end, the shape of the simulation box (side lengths and angles) are allowed to change by a means of a transformation of the space of coordinates and an appropriate acceptance rule for the volume moves [4]. The transformation of coordinates can be operated as follows:

$$\mathbf{r}_i = H\mathbf{s}_i \tag{1}$$

where H is a matrix whose columns are the vectors that define the edges of the simulation box, $\mathbf{r}_i$ are the coordinates in the real space and $\mathbf{s}_i$ are the coordinates in a cube of size 1. Conveniently, the volume of the system is then the determinant of this matrix ($V = \det H$), therefore we assume it to be $\det H > 0$. During each try to change volume, a random element of the matrix H is changed to explore the phase space of the system. To compute the acceptance probability of each try we use the function W defined as follows [5]:

$$W = \Delta U + P\Delta V - N\kappa_B T\Delta(\log V) \tag{2}$$

where U is the total energy of the pairs interactions, V the volume, N the number of particles, κ_B the Boltzmann constant and T the temperature. Then, the acceptance probability acc can be expressed like:

$$acc = \quad 1 \quad if \quad W \leq 0$$

$$acc = \quad \exp(-W/\kappa_B T) \quad if \quad W > 0$$

In order to correctly implement these transformations into a simulation code, we need to carefully address every calculation regarding distances, specially when working with anisotropic particles whose relative distance relies on their relative orientation. Meanwhile, the latter is naturally performed in the real space (r_i). Any algorithm relying on the adjacency of particles, like the ones dealing with periodic boundary conditions or a cell lists, should use s_i particle coordinates. This transformation might change orientations of anisotropic particles in s_i coordinates, but will behave as usual in the space of r_i coordinates.

The Isobaric-Isothermal ensemble (NPT) implementation can be understood as a simplification of the isotension-isothermal ensemble, where only the diagonal elements of H matrix are varied starting from an orthogonal shape only varying the elements H_{11}, H_{22} and H_{33}, which would represent the sides of the simulation box (for more details on this see reference [4]).

CALCULATION OF NEMATIC AND CUBATIC ORDER PARAMETER AND CORRELATION FUNCTION

To classify the phases reported in the article, several correlation functions and order parameters have been calculated. The long-range orientation order was determined by the standard procedure of diagonalization of the following second rank symmetric tensor [6]:

$$Q_{\alpha\beta} = \frac{1}{2N}\langle \sum_{1}^{N}(3\hat{\mathbf{u}}_{i\alpha}\cdot\hat{\mathbf{u}}_{i\beta} - \delta_{\alpha\beta})\rangle \tag{3}$$

where i indicates a generic particle, $\hat{u}_i$ denotes its unit orientation vector and α and β indicate the components of the vector. $\delta_{\alpha\beta}$ is the delta Kronecker. The nematic order parameter, S_2, is the largest eigenvalue resulting from the diagonalization of this tensor, while the nematic director vector that defines the preferred orientation of the particles is its associated eigenvector.

The cubatic order parameter has been calculated following the procedure proposed by Duncan and coworkers [7]. The starting point of the method is the definition of a four-rank tensor

$$Q_{\alpha\beta\gamma\delta} = \frac{35}{8}u_\alpha u_\beta u_\gamma u_\delta - \frac{5}{8}(u_\alpha u_\beta \delta_{\gamma\delta} + u_\alpha u_\gamma \delta_{\beta\delta} + u_\alpha u_\delta \delta_{\beta\gamma} + u_\beta u_\gamma \delta_{\alpha\delta} + u_\beta u_\delta \delta_{\alpha\gamma} + u_\gamma u_\delta \delta_{\alpha\beta}) + \frac{1}{8}(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) \tag{4}$$

The cubatic order parameter, S_{cub} can be calculated solving the tensor equation

$$Q_{\alpha\beta\gamma\delta}Q_{\alpha\beta} = \frac{7S_4}{8}Q_{\gamma\delta} \tag{5}$$

where a second-rank tensor $Q_{\alpha\beta}$ is defined. This tensor is symmetric and traceless. Due to these properties, and the symmetries on $Q_{\alpha\beta\gamma\delta}$, this tensor equation can be reduced to five coupled equations for $(\alpha,\beta) = (x,x),(x,y),(x,z),(y,y)$ and (y,z). From the diagonalization of the matrix associated to this system of equations S_{cub} can be calculated as $S_4 = 8/7\Gamma$, with Γ the largest eigenvalue resulting from the referred diagonalization.

In a perfect cubatic phase (where the particles are oriented with the same probability in three mutually perpendicular directions) the cubatic order paramter takes the value $S_{cub} = 1$, while it trends to $S_{cub} = 0$ in an isotropic phase. In phases with high level of orientational alignment, as in nematic or columnar phases, S_{cub} becomes larger than 1.

To characterize phases and structures with some degree of positional order, a list of correlation function have been calculated. For instance, the pair correlation function parallel to the nematic director, that informs about the possibility of arranging the particles in layers perpendicular to the nematic director, is defined as:

$$g_\parallel(r_\parallel) = \frac{1}{N_p \rho S_\parallel}\left\langle \sum_i \sum_{j\neq i} \delta(r_\parallel - r_{\parallel,ij}) \right\rangle \tag{6}$$

where $\rho = N_p/V$, N_p is the number of particles, V the box volume, δ is the Dirac delta. $r_{\parallel,ij}$ is the projection on the nematic director of the distance between particles i and j. $S_\parallel$ is the surface of a plane at a distance $r_\parallel$ in the direction of the nematic director from the particle, i bounded by a sphere with radius half of the shorter side of the simulation box. $g^0_\parallel(r_\parallel)$ is similar to the previous one, but restricted to particles i and j with a perpendicular distance to the nematic director shorter than $0.5/L + \sigma$. This correlation function provides information about correlation to particles that belong to the same column.

The pair correlation function perpendicular to the nematic director gives information about columnar packing. It is defined as:

$$g_\perp(r_\perp) = \frac{1}{N_p \rho S_\perp}\left\langle \sum_i \sum_{j\neq i} \delta(r_\perp - r_{\perp,ij}) \right\rangle \tag{7}$$

where now $r_{\perp,ij}$ is the projection perpendicular to the nematic director of the distance between particles i and j. $S_\perp$ is the surface of a plane at a distance $r_\perp$ in the direction perpendicular to the nematic director from the particle i bounded by an sphere with radius half of the shorter side of the simulation box.

The orientational correlation function is defined as the average, for each intermolecular distance, of the second Legendre polynomial of the cosine of the angle between the orientation of the particles, $g_2(r) = P_2(\hat{u}_i \cdot \hat{u}_i)$. This function give information about the averaged relative orientation of particles separated a distance r. g_2 tends to one if the particles have similar orientation, -0.5 if they are perpendicular and 0 if on average the particles are randomly oriented.

The angular distribution of the projection of the vector director of the particles in the plane perpendicular to the nematic director $h(\varphi)$ is calculated as:

$$h(\varphi) = \frac{1}{N_p}\left\langle \sum_i \delta(\varphi - \varphi_i) \right\rangle \tag{8}$$

being φ_i is the azimuthal angle of the representation of the vector $\hat{u}_i$ in spherical coordinates with respect to a

reference system with the z-axis in the direction of the nematic director vector.

EVOLUTION OF THE CUBATIC ORDER PARAMETER IN ISOTHERMS WITH CUBATIC PHASE

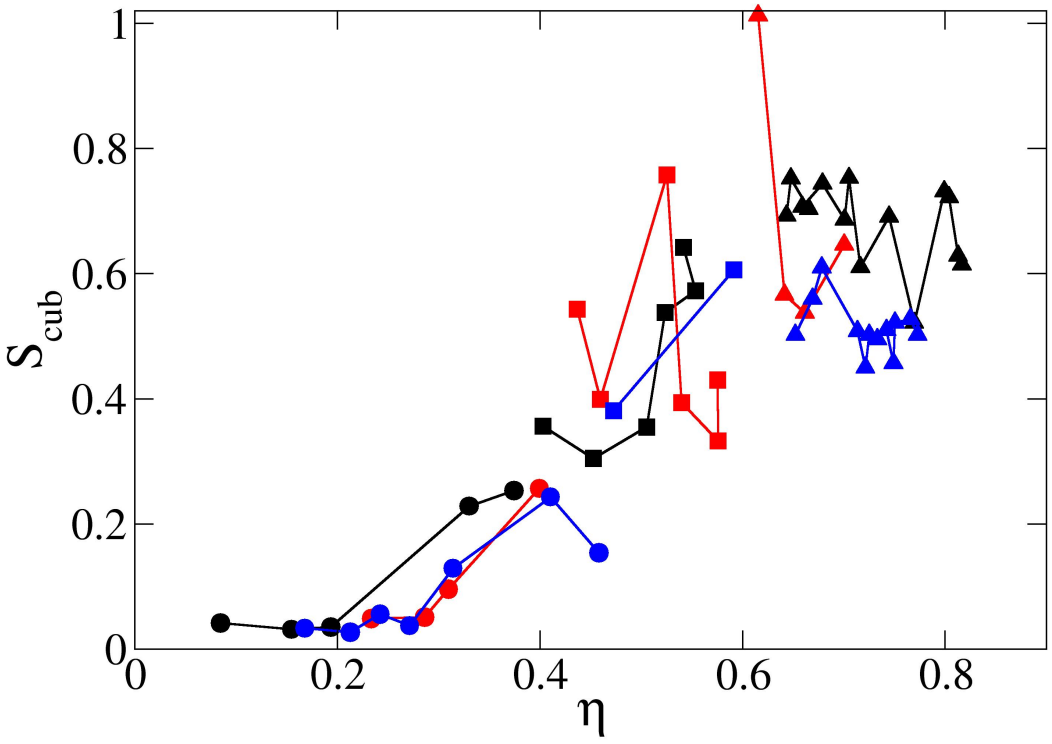

FIG. 1. Evolution of the cubatic order parameter for the U_{Cs} model at $T^* = 0.5$ (black lines and symbols), $T^* = 1$ (read lines and symbols) and the U_{Cw} model at $T^* = 1$ (blue lines and symbols). Circles, squares and triangles correspond to states points in the I, Q and C_t phase respectively.

TABLES

TABLE I. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Fs} model described in the main text at $T^* = k_B T/\epsilon_0 = 5.85$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/11.7$.

P^*	η	S_2	Phase/Structure
75	0.199(2)	0.036(7)	I
100	0.230(2)	0.140(5)	I
140	0.281(2)	0.509(2)	N
180	0.324(3)	0.709(7)	N
200	0.339(2)	0.717(7)	N
225	0.359(3)	0.783(8)	N
250	0.375(3)	0.761(6)	N
275	0.392(3)	0.802(1)	N
300	0.409(3)	0.863(4)	N
325	0.420(3)	0.715(7)	N
350	0.434(3)	0.755(9)	N
375	0.448(3)	0.824(5)	N
400	0.463(3)	0.761(5)	N
450	0.541(4)	0.960(2)	C_d
500	0.568(4)	0.956(3)	C_d
600	0.609(4)	0.976(4)	C_o
700	0.644(3)	0.989(1)	C_o
800	0.667(3)	0.984(2)	C_o
900	0.693(4)	0.996(3)	C_o
1000	0.711(4)	0.997(3)	C_o
1250	0.748(3)	0.998(9)	C_o
1500	0.770(3)	0.999(5)	C_o
1750	0.785(3)	0.999(3)	C_o
2000	0.792(4)	0.994(5)	C_o
2250	0.800(2)	0.973(4)	C_t
2500	0.808(2)	0.948(2)	C_t
2750	0.817(2)	0.961(2)	C_t
3000	0.823(2)	0.930(3)	C_t
3250	0.830(2)	0.924(1)	C_t
3500	0.837(2)	0.942(2)	C_t
4000	0.847(2)	0.912(3)	C_t
5000	0.865(1)	0.903(2)	C_t
6000	0.880(2)	0.912(1)	C_t

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TABLE II. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Fs} model described in the main text at $T^* = k_B T/\epsilon_0 = 11.7$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/11.7$.

P^*	η	S_2	Phase/Structure
100	0.162(5)	0.031(8)	I
200	0.228(1)	0.057(1)	I
250	0.257(2)	0.232(2)	I
300	0.284(2)	0.333(5)	I
350	0.314(2)	0.602(8)	N
400	0.339(2)	0.716(3)	N
450	0.359(2)	0.783(6)	N
500	0.380(4)	0.826(4)	N
550	0.392(4)	0.842(6)	N
600	0.408(2)	0.873(3)	N
650	0.421(2)	0.843(1)	N
700	0.435(3)	0.878(6)	N
750	0.446(3)	0.874(1)	N
800	0.458(3)	0.821(6)	N
850	0.471(3)	0.923(3)	N
900	0.512(4)	0.922(3)	C_d
1000	0.556(4)	0.956(2)	C_d
1200	0.603(4)	0.965(2)	C_d
1500	0.649(4)	0.978(2)	C_o
2000	0.702(3)	0.966(7)	C_o
2500	0.738(2)	0.980(3)	C_o
3000	0.766(3)	0.989(3)	C_o
3500	0.787(3)	0.991(2)	C_o
4000	0.805(3)	0.991(3)	C_o
4500	0.819(3)	0.992(1)	C_o
5500	0.842(2)	0.987(2)	C_o
6000	0.851(2)	0.980(2)	C_t
7000	0.866(2)	0.954(2)	C_t

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TABLE III. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Fs} model described in the main text at $T^* = k_B T/\epsilon_0 = 23.4$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/11.7$.

P^*	η	S_2	Phase/Structure
50	0.080(4)	0.032(1)	I
200	0.164(3)	0.043(1)	I
300	0.197(4)	0.041(8)	I
550	0.275(7)	0.292(2)	I
620	0.295(5)	0.541(1)	N
670	0.307(3)	0.531(2)	N
800	0.344(3)	0.721(8)	N
850	0.356(3)	0.749(1)	N
900	0.361(4)	0.764(9)	N
1200	0.415(3)	0.869(4)	N
1300	0.432(2)	0.868(1)	N
1400	0.444(3)	0.904(5)	N
1500	0.454(3)	0.890(5)	N
1700	0.479(3)	0.905(9)	N
1900	0.531(4)	0.933(4)	N
2200	0.583(4)	0.960(3)	C_d
2500	0.617(4)	0.966(3)	C_d
3000	0.658(4)	0.971(2)	C_o
3500	0.690(4)	0.974(2)	C_o
4000	0.716(4)	0.970(3)	C_o
4500	0.737(3)	0.980(1)	C_o
5000	0.755(3)	0.967(7)	C_o
5500	0.771(3)	0.972(2)	C_o
6000	0.786(3)	0.978(3)	C_o
6500	0.798(3)	0.982(2)	C_o
7000	0.810(3)	0.986(3)	C_o
8000	0.830(3)	0.985(1)	C_o
9000	0.846(3)	0.981(3)	C_o
10000	0.861(2)	0.988(1)	C_o
11000	0.874(2)	0.989(8)	C_o
12500	0.889(2)	0.977(2)	C_o

TABLE IV. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Fw} model described in the main text at $T^* = k_BT/\epsilon_0 = 1.375$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/2.75$.

P^*	η	S_2	Phase/Structure
15	0.203(4)	0.062(9)	I
20	0.234(2)	0.102(9)	I
30	0.293(2)	0.474(8)	N
34	0.315(3)	0.640(2)	N
41	0.345(3)	0.750(7)	N
45	0.351(2)	0.638(4)	N
50	0.374(2)	0.788(3)	N
55	0.387(2)	0.789(7)	N
60	0.402(3)	0.784(3)	N
63	0.407(2)	0.803(3)	N
67	0.419(3)	0.775(3)	N
74	0.433(2)	0.727(5)	N
80	0.452(3)	0.717(5)	N
81	0.467(2)	0.807(4)	N
82	0.512(4)	0.874(6)	N
83	0.540(3)	0.930(10)	N
85	0.580(4)	0.971(2)	C_d
87	0.587(4)	0.967(7)	C_d
92	0.603(4)	0.979(1)	C_d
95	0.608(4)	0.980(2)	C_o
99	0.617(4)	0.981(2)	C_o
107	0.633(3)	0.983(1)	C_o
115	0.645(3)	0.985(1)	C_o
125	0.658(3)	0.987(7)	C_o
136	0.672(3)	0.986(5)	C_o
143	0.681(3)	0.986(4)	C_o
150	0.691(3)	0.987(4)	C_o
155	0.688(3)	0.988(7)	C_o
160	0.691(3)	0.989(8)	C_o
165	0.695(3)	0.986(5)	C_o
175	0.706(3)	0.989(6)	C_o
200	0.717(2)	0.974(10)	C_o
300	0.752(2)	0.878(1)	C_t
350	0.765(2)	0.895(3)	C_t
400	0.776(2)	0.886(1)	C_t
450	0.785(2)	0.853(1)	C_t
500	0.793(2)	0.844(7)	C_t
550	0.802(2)	0.889(2)	C_t
600	0.807(2)	0.855(7)	C_t
800	0.829(1)	0.801(2)	C_t
1000	0.847(1)	0.832(5)	C_t
1300	0.866(1)	0.799(2)	C_t
1500	0.878(1)	0.834(2)	C_t
2000	0.899(1)	0.816(1)	C_t
2500	0.916(1)	0.805(7)	C_t

TABLE V. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Fw} model described in the main text at $T^* = k_B T/\epsilon_0 = 2.75$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/2.75$.

P^*	η	S_2	Phase/Structure
33	0.196(7)	0.036(7)	I
37	0.209(1)	0.023(9)	I
45	0.229(2)	0.047(7)	I
53	0.248(1)	0.047(1)	I
72	0.305(2)	0.682(3)	N
86	0.330(2)	0.712(7)	N
128	0.394(3)	0.847(7)	N
140	0.408(2)	0.841(2)	N
161	0.432(3)	0.859(8)	N
175	0.446(2)	0.803(1)	N
180	0.455(2)	0.715(9)	N
190	0.480(3)	0.871(9)	N
200	0.528(3)	0.921(4)	C_d
210	0.547(4)	0.958(3)	C_d
220	0.562(4)	0.963(2)	C_d
230	0.572(4)	0.962(2)	C_d
250	0.594(3)	0.965(3)	C_d
275	0.615(3)	0.971(1)	C_d
300	0.634(3)	0.974(2)	C_o
336	0.657(3)	0.981(7)	C_o
350	0.665(3)	0.983(9)	C_o
375	0.677(3)	0.984(8)	C_o
400	0.689(3)	0.986(2)	C_o
450	0.708(3)	0.988(7)	C_o
500	0.725(3)	0.988(1)	C_o
550	0.741(3)	0.987(9)	C_o
600	0.753(3)	0.988(7)	C_o
700	0.770(3)	0.942(8)	C_t
800	0.786(2)	0.936(5)	C_t
900	0.800(2)	0.914(8)	C_t
1000	0.811(2)	0.936(1)	C_t
1200	0.831(2)	0.955(2)	C_t
1500	0.851(2)	0.911(3)	C_t
2000	0.878(2)	0.867(2)	C_t
2500	0.898(1)	0.880(2)	C_t

TABLE VI. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Fw} model described in the main text at $T^* = k_B T/\epsilon_0 = 5.5$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/2.75$.

P^*	η	S_2	Phase/Structure
55	0.176(2)	0.036(1)	I
65	0.192(2)	0.038(8)	I
70	0.200(2)	0.033(9)	I
75	0.205(2)	0.038(1)	I
100	0.236(1)	0.047(2)	I
125	0.266(2)	0.257(9)	I
150	0.302(3)	0.524(2)	N
175	0.326(2)	0.703(5)	N
250	0.388(3)	0.845(8)	N
280	0.406(3)	0.859(6)	N
320	0.429(3)	0.887(4)	N
371	0.456(3)	0.859(6)	N
399	0.469(3)	0.864(8)	N
415	0.526(4)	0.938(3)	C_d
430	0.536(3)	0.955(3)	C_d
450	0.551(4)	0.957(3)	C_d
470	0.563(4)	0.956(2)	C_d
500	0.580(4)	0.958(2)	C_d
600	0.624(4)	0.973(2)	C_d
700	0.657(4)	0.977(1)	C_o
864	0.697(4)	0.979(2)	C_o
892	0.704(3)	0.980(1)	C_o
971	0.720(3)	0.979(3)	C_o
999	0.725(3)	0.978(1)	C_o
1200	0.756(3)	0.989(9)	C_o
1300	0.769(3)	0.987(2)	C_o
1500	0.792(3)	0.988(2)	C_o
2000	0.834(3)	0.987(7)	C_o

TABLE VII. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Es} model described in the main text at $T^* = k_B T/\epsilon_0 = 5.65$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/11.3$.

P^*	η	S_2	Phase/Structure
51	0.172(2)	0.036(1)	I
54	0.177(2)	0.058(2)	I
70	0.207(3)	0.287(4)	I
90	0.299(6)	0.900(8)	N
110	0.367(3)	0.964(1)	N
130	0.404(4)	0.977(1)	N
140	0.421(4)	0.983(6)	N
150	0.435(3)	0.984(1)	N
160	0.445(6)	0.984(1)	N
180	0.489(4)	0.984(5)	N
200	0.530(4)	0.981(1)	N
225	0.580(5)	0.997(1)	S
250	0.630(2)	0.997(7)	S
275	0.639(3)	0.996(1)	S
375	0.649(3)	0.997(10)	S
400	0.771(3)	0.998(10)	C_o
420	0.778(3)	0.998(7)	C_o
450	0.785(3)	0.999(8)	C_o
500	0.794(3)	0.999(7)	C_o
550	0.804(3)	0.999(7)	C_o
650	0.819(3)	0.999(7)	C_o
700	0.825(3)	0.999(5)	C_o
750	0.831(3)	0.999(5)	C_o
800	0.837(2)	0.999(5)	C_o
900	0.847(2)	0.999(4)	C_o

TABLE VIII. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Es} model described in the main text at $T^* = k_BT/\epsilon_0 = 11.3$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/11.3$.

P^*	η	S_2	Phase/Structure
90	0.161(1)	0.037(1)	I
110	0.175(2)	0.036(8)	I
250	0.265(1)	0.195(6)	I
390	0.365(3)	0.895(3)	N
550	0.427(7)	0.962(2)	N
600	0.446(3)	0.966(1)	N
650	0.463(3)	0.970(2)	N
700	0.477(3)	0.976(2)	N
725	0.635(6)	0.992(4)	C_d
750	0.655(6)	0.993(5)	C_d
900	0.712(5)	0.995(2)	C_o
1000	0.734(4)	0.996(2)	C_o
1200	0.768(4)	0.997(2)	C_o
1500	0.805(4)	0.998(2)	C_o
2500	0.878(2)	0.999(6)	C_o
2800	0.892(2)	0.999(6)	C_o
3300	0.913(2)	0.999(5)	C_o

TABLE IX. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Es} model described in the main text at $T^* = k_BT/\epsilon_0 = 22.6$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/11.3$.

P^*	η	S_2	Phase/Structure
200	0.167(2)	0.023(7)	I
340	0.216(2)	0.039(10)	I
400	0.232(1)	0.044(2)	I
430	0.243(10)	0.105(4)	I
550	0.276(3)	0.235(4)	I
610	0.296(2)	0.471(3)	N
850	0.359(6)	0.757(1)	N
950	0.376(3)	0.838(4)	N
1000	0.385(3)	0.844(1)	N
1100	0.403(3)	0.861(6)	N
1200	0.418(3)	0.875(7)	N
1300	0.432(3)	0.901(4)	N
1400	0.446(3)	0.811(10)	N
1500	0.464(3)	0.939(3)	N
1600	0.554(6)	0.967(2)	C_d
1700	0.580(4)	0.971(1)	C_d
1900	0.629(5)	0.985(9)	C_d
2200	0.682(5)	0.989(9)	C_d
2500	0.724(5)	0.992(5)	C_o
3000	0.774(4)	0.995(4)	C_o
3500	0.810(4)	0.996(3)	C_o
4000	0.839(4)	0.997(2)	C_o

TABLE X. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Ew} model described in the main text at $T^* = k_BT/\epsilon_0 = 1.115$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/2.23$.

P^*	η	S_2	Phase/Structure
7	0.157(2)	0.032(9)	I
11	0.212(4)	0.439(4)	N
13	0.264(4)	0.744(1)	N
17	0.321(3)	0.874(5)	N
19	0.340(3)	0.895(3)	N
21	0.361(3)	0.911(2)	N
23	0.378(4)	0.935(5)	N
25	0.386(3)	0.940(2)	N
27	0.399(3)	0.945(2)	N
29	0.408(4)	0.948(2)	N
31	0.418(3)	0.950(1)	N
33	0.427(3)	0.960(2)	N
35	0.438(3)	0.964(1)	N
37	0.439(3)	0.941(5)	N
39	0.454(3)	0.968(2)	N
41	0.461(2)	0.967(1)	N
43	0.467(3)	0.971(1)	N
45	0.475(3)	0.968(10)	N
48	0.485(3)	0.979(1)	N
51	0.500(3)	0.982(6)	N
54	0.506(4)	0.982(1)	N
57	0.523(5)	0.987(1)	N
60	0.536(4)	0.989(8)	N
63	0.693(3)	0.992(3)	C_o
66	0.701(3)	0.992(2)	C_o
69	0.706(3)	0.992(3)	C_o
75	0.709(3)	0.992(3)	C_o
80	0.719(3)	0.991(3)	C_o
85	0.720(3)	0.992(2)	C_o
90	0.726(2)	0.991(2)	C_o
95	0.731(3)	0.991(2)	C_o
100	0.735(2)	0.992(2)	C_o
110	0.739(2)	0.993(2)	C_o
120	0.747(2)	0.993(2)	C_o
130	0.755(2)	0.992(4)	C_o
140	0.759(2)	0.993(2)	C_o
150	0.764(2)	0.992(2)	C_o
160	0.769(2)	0.993(2)	C_o
180	0.777(2)	0.993(2)	C_o
200	0.785(2)	0.993(2)	C_o
225	0.793(2)	0.994(2)	C_o
250	0.801(2)	0.994(2)	C_o
275	0.806(2)	0.973(3)	C_o
300	0.814(2)	0.994(2)	C_o
325	0.820(2)	0.990(2)	C_o
350	0.826(2)	0.992(2)	C_o
375	0.831(2)	0.992(2)	C_o
400	0.835(2)	0.981(3)	C_o
500	0.851(2)	0.989(4)	C_o
600	0.861(1)	0.986(5)	C_o
700	0.869(3)	0.896(4)	C_t

TABLE XI. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Ew} model described in the main text at $T^* = k_B T/\epsilon_0 = 2.23$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/2.23$.

P^*	η	S_2	Phase/Structure
33	0.224(3)	0.251(6)	I
39	0.251(3)	0.459(3)	N
50	0.298(2)	0.720(5)	N
66	0.347(3)	0.864(5)	N
81	0.380(3)	0.894(3)	N
95	0.404(3)	0.924(3)	N
100	0.414(2)	0.936(2)	N
110	0.425(2)	0.926(3)	N
120	0.440(3)	0.926(5)	N
140	0.469(3)	0.963(2)	N
160	0.563(4)	0.983(7)	N
180	0.643(4)	0.989(7)	C_d
200	0.669(4)	0.991(5)	C_o
220	0.687(4)	0.993(6)	C_o
240	0.702(3)	0.993(5)	C_o
260	0.715(3)	0.994(4)	C_o
280	0.727(3)	0.993(5)	C_o
300	0.738(3)	0.994(4)	C_o
330	0.752(3)	0.994(6)	C_o
360	0.765(3)	0.994(3)	C_o
390	0.774(3)	0.993(5)	C_o
420	0.784(3)	0.993(3)	C_o
450	0.791(2)	0.994(4)	C_o
500	0.803(3)	0.995(2)	C_o
550	0.813(2)	0.994(3)	C_o
600	0.823(2)	0.994(2)	C_o
650	0.831(2)	0.994(2)	C_o
700	0.838(2)	0.994(4)	C_o
750	0.845(2)	0.994(3)	C_o
800	0.852(2)	0.993(4)	C_o
1200	0.884(1)	0.919(5)	C_t

TABLE XII. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Ew} model described in the main text at $T^* = k_B T/\epsilon_0 = 4.46$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/2.23$.

P^*	η	S_2	Phase/Structure
60	0.162(8)	0.285(1)	I
71	0.174(9)	0.303(5)	I
80	0.181(1)	0.364(5)	I
140	0.336(3)	0.796(6)	N
150	0.343(3)	0.802(6)	N
160	0.353(2)	0.813(8)	N
170	0.366(3)	0.862(7)	N
180	0.374(3)	0.855(5)	N
200	0.390(3)	0.869(8)	N
220	0.407(3)	0.903(4)	N
240	0.420(3)	0.901(5)	N
260	0.435(3)	0.910(4)	N
280	0.448(3)	0.921(4)	N
300	0.461(3)	0.939(2)	N
320	0.524(4)	0.956(4)	C_d
340	0.550(4)	0.970(2)	C_d
360	0.568(4)	0.972(2)	C_d
380	0.587(4)	0.974(1)	C_d
400	0.603(4)	0.980(3)	C_d
430	0.623(4)	0.980(1)	C_d
460	0.642(4)	0.983(1)	C_o
490	0.658(4)	0.985(8)	C_o
520	0.674(4)	0.988(1)	C_o
550	0.688(4)	0.988(8)	C_o
580	0.700(4)	0.990(8)	C_o
610	0.711(4)	0.990(6)	C_o
640	0.722(4)	0.992(7)	C_o
670	0.731(3)	0.991(6)	C_o
700	0.740(4)	0.992(8)	C_o
730	0.748(3)	0.993(5)	C_o
750	0.754(4)	0.993(7)	C_o
800	0.765(4)	0.993(6)	C_o
850	0.776(4)	0.994(6)	C_o
900	0.786(4)	0.995(4)	C_o
950	0.795(4)	0.994(5)	C_o
1000	0.803(3)	0.994(5)	C_o
1100	0.819(3)	0.995(4)	C_o
1200	0.832(3)	0.995(3)	C_o
1300	0.844(3)	0.995(5)	C_o
1500	0.861(4)	0.984(2)	C_o

TABLE XIII. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Cs} model described in the main text at $T^* = k_BT/\epsilon_0 = 0.5$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/1$.

P^*	η	S_2	Phase/Structure
1	0.085(1)	0.021(6)	I
3	0.153(2)	0.021(7)	I
5	0.193(2)	0.021(8)	I
6	0.327(1)	0.075(5)	I
7	0.376(2)	0.089(1)	I
9	0.406(3)	0.138(5)	Q
11	0.456(3)	0.131(3)	Q
12	0.471(2)	0.107(4)	Q
14	0.504(3)	0.037(6)	Q
17	0.527(2)	0.055(5)	Q
20	0.557(2)	0.052(3)	Q
24	0.639(3)	0.206(4)	C_t
26	0.655(4)	0.210(7)	C_t
28	0.666(4)	0.207(6)	C_t
30	0.661(3)	0.234(5)	C_t
32	0.679(2)	0.254(4)	C_t
36	0.708(2)	0.237(4)	C_t
43	0.723(3)	0.246(5)	C_t
50	0.743(3)	0.254(7)	C_t
80	0.798(2)	0.285(5)	C_t
86	0.805(2)	0.280(5)	C_t
93	0.812(2)	0.286(3)	C_t
100	0.820(2)	0.297(5)	C_t
150	0.862(2)	0.339(6)	C_t
200	0.896(2)	0.371(8)	C_t
250	0.919(2)	0.406(7)	C_t
300	0.939(2)	0.438(2)	C_t
400	0.972(2)	0.486(1)	C_t

TABLE XIV. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Cs} model described in the main text at $T^* = k_BT/\epsilon_0 = 1.0$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/1$.

P^*	η	S_2	Phase/Structure
17	0.231(3)	0.053(1)	I
25	0.282(2)	0.062(3)	I
30	0.310(3)	0.224(3)	I
43	0.403(4)	0.326(3)	I
45	0.444(3)	0.348(1)	Q
47	0.464(4)	0.250(1)	Q
50	0.529(3)	0.227(4)	Q
55	0.541(3)	0.093(4)	Q
60	0.574(4)	0.100(7)	Q
65	0.585(4)	0.148(10)	Q
80	0.641(3)	0.386(3)	C_t
90	0.670(3)	0.388(2)	C_t
100	0.699(3)	0.367(4)	C_t
120	0.737(3)	0.367(5)	C_t
136	0.762(3)	0.381(1)	C_t
150	0.779(3)	0.379(7)	C_t
170	0.801(3)	0.429(2)	C_t
190	0.820(3)	0.440(4)	C_t
210	0.837(3)	0.444(2)	C_t
220	0.844(3)	0.443(3)	C_t
236	0.855(3)	0.432(4)	C_t
250	0.864(3)	0.444(6)	C_t
300	0.893(2)	0.465(9)	C_t
400	0.935(2)	0.529(9)	C_t
900	1.034(2)	0.540(1)	C_t

TABLE XV. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Cs} model described in the main text at $T^* = k_BT/\epsilon_0 = 2.0$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/1$.

P^*	η	S_2	Phase/Structure
25	0.197(2)	0.033(9)	I
30	0.216(2)	0.059(9)	I
40	0.251(2)	0.175(3)	I
67	0.339(3)	0.635(1)	N
80	0.373(3)	0.743(2)	N
99	0.417(3)	0.816(7)	N
127	0.473(3)	0.785(3)	N
130	0.482(3)	0.660(8)	N
146	0.544(5)	0.742(8)	N
150	0.559(5)	0.905(4)	C_d
155	0.569(4)	0.894(2)	C_d
160	0.600(4)	0.702(2)	C_d
170	0.615(5)	0.883(5)	C_d
174	0.614(4)	0.943(6)	C_d
180	0.635(4)	0.822(7)	C_d
200	0.663(4)	0.897(6)	C_d
220	0.704(4)	0.623(8)	C_d
248	0.735(4)	0.635(2)	C_t
262	0.751(4)	0.657(1)	C_t
276	0.764(4)	0.691(2)	C_t
280	0.767(4)	0.673(4)	C_t
290	0.773(3)	0.645(6)	C_t
310	0.793(3)	0.609(4)	C_t
350	0.823(4)	0.605(1)	C_t

TABLE XVI. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Cw} model described in the main text at $T^* = k_BT/\epsilon_0 = 0.5$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/1$.

P^*	η	S_2	Phase/Structure
3	0.165(2)	0.027(1)	I
5	0.209(2)	0.047(2)	I
7	0.242(3)	0.155(3)	I
9	0.271(2)	0.193(3)	I
11	0.321(4)	0.268(2)	I
13	0.416(3)	0.152(1)	I
15	0.462(2)	0.104(7)	I
19	0.477(2)	0.132(5)	Q
21	0.591(3)	0.294(3)	Q
23	0.626(3)	0.297(7)	C_t
25	0.638(3)	0.299(4)	C_t
27	0.649(3)	0.309(5)	C_t
29	0.660(3)	0.319(5)	C_t
31	0.664(3)	0.312(5)	C_t
33	0.671(3)	0.313(3)	C_t
35	0.679(2)	0.322(7)	C_t
37	0.681(2)	0.332(3)	C_t
39	0.691(2)	0.320(5)	C_t
41	0.692(2)	0.336(10)	C_t
43	0.700(2)	0.326(4)	C_t
45	0.698(2)	0.330(3)	C_t
48	0.708(2)	0.329(3)	C_t
51	0.715(2)	0.346(5)	C_t
54	0.718(2)	0.337(6)	C_t
57	0.721(2)	0.344(3)	C_t
60	0.725(2)	0.346(4)	C_t
63	0.733(2)	0.344(8)	C_t
66	0.732(2)	0.379(5)	C_t
69	0.739(2)	0.353(5)	C_t
75	0.746(2)	0.372(4)	C_t
80	0.751(2)	0.362(4)	C_t
85	0.758(2)	0.385(3)	C_t
90	0.765(2)	0.383(3)	C_t
95	0.767(2)	0.407(4)	C_t
100	0.772(2)	0.407(6)	C_t
110	0.780(2)	0.420(4)	C_t
120	0.788(2)	0.425(4)	C_t
130	0.796(2)	0.437(4)	C_t
140	0.801(2)	0.440(6)	C_t
150	0.809(2)	0.463(6)	C_t
160	0.814(2)	0.459(5)	C_t
180	0.824(2)	0.484(3)	C_t
200	0.834(2)	0.493(4)	C_t
250	0.855(1)	0.536(3)	C_t
275	0.865(1)	0.570(4)	C_t
300	0.873(2)	0.584(5)	C_t
325	0.881(1)	0.598(2)	C_t
350	0.888(1)	0.632(5)	C_t
375	0.895(1)	0.639(6)	C_t
400	0.901(1)	0.641(3)	C_t
500	0.922(1)	0.680(3)	C_t

TABLE XVII. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Cw} model described in the main text at $T^* = k_BT/\epsilon_0 = 1.0$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/1$.

P^*	η	S_2	Phase/Structure
10	0.189(4)	0.036(9)	I
15	0.223(2)	0.053(1)	I
18	0.243(2)	0.061(3)	I
21	0.263(2)	0.195(4)	I
24	0.283(2)	0.367(2)	I
27	0.299(2)	0.404(4)	N
30	0.317(2)	0.503(9)	N
33	0.333(2)	0.537(2)	N
36	0.345(3)	0.565(2)	N
39	0.359(2)	0.597(1)	N
42	0.372(3)	0.564(9)	N
45	0.384(2)	0.532(7)	N
48	0.402(3)	0.533(6)	N
57	0.482(3)	0.279(2)	C_d
60	0.494(6)	0.290(8)	C_d
63	0.511(3)	0.257(2)	C_d
66	0.555(4)	0.464(4)	C_t
69	0.566(4)	0.452(1)	C_t
72	0.598(4)	0.459(10)	C_t
75	0.616(3)	0.427(2)	C_t
78	0.623(3)	0.420(9)	C_t
81	0.630(3)	0.431(8)	C_t
85	0.641(3)	0.446(10)	C_t
90	0.651(3)	0.431(6)	C_t
95	0.663(3)	0.443(8)	C_t
100	0.672(3)	0.443(6)	C_t
110	0.688(3)	0.440(9)	C_t
120	0.702(3)	0.457(8)	C_t
140	0.727(3)	0.463(5)	C_t
160	0.748(3)	0.476(7)	C_t
180	0.765(3)	0.509(7)	C_t
200	0.780(2)	0.543(6)	C_t
220	0.793(2)	0.564(8)	C_t
240	0.804(2)	0.573(5)	C_t
260	0.814(2)	0.601(7)	C_t
280	0.823(2)	0.598(6)	C_t
300	0.832(2)	0.619(10)	C_t
330	0.845(2)	0.662(9)	C_t
360	0.856(2)	0.691(5)	C_t
390	0.867(2)	0.712(3)	C_t
420	0.875(2)	0.715(8)	C_t
500	0.898(2)	0.769(2)	C_t
1000	0.958(2)	0.629(8)	C_t

TABLE XVIII. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Cw} model described in the main text at $T^* = k_BT/\epsilon_0 = 2.0$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/1$.

P^*	η	S_2	Phase/Structure
35	0.232(2)	0.056(3)	I
45	0.265(2)	0.249(2)	I
55	0.300(2)	0.536(3)	N
65	0.325(2)	0.590(2)	N
85	0.374(3)	0.779(2)	N
100	0.402(3)	0.816(7)	N
110	0.420(3)	0.765(8)	N
120	0.438(3)	0.736(1)	N
130	0.457(3)	0.725(6)	N
140	0.477(3)	0.725(4)	N
150	0.538(4)	0.920(7)	C_d
160	0.563(4)	0.918(3)	C_d
170	0.583(4)	0.912(5)	C_d
180	0.598(4)	0.923(3)	C_d
200	0.632(4)	0.887(3)	C_d
220	0.659(4)	0.851(6)	C_t
240	0.684(4)	0.829(1)	C_t
260	0.701(3)	0.824(7)	C_t
280	0.720(3)	0.790(7)	C_t
300	0.735(3)	0.817(2)	C_t
320	0.748(3)	0.790(3)	C_t
340	0.760(3)	0.799(1)	C_t
360	0.773(3)	0.812(3)	C_t
380	0.784(3)	0.812(6)	C_t
400	0.793(3)	0.795(5)	C_t
430	0.806(3)	0.824(9)	C_t
460	0.820(3)	0.847(8)	C_t
490	0.830(3)	0.856(4)	C_t
520	0.841(3)	0.841(4)	C_t
550	0.853(3)	0.892(5)	C_t
570	0.856(3)	0.854(8)	C_t
580	0.860(3)	0.881(10)	C_t
610	0.871(2)	0.915(5)	C_t
800	0.905(4)	0.840(2)	C_t

TABLE XIX. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Ts} model described in the main text at $T^* = k_B T/\epsilon_0 = 4.35$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/8.66$.

P^*	η	S_2	Phase/Structure
15	0.104(10)	0.020(7)	I
25	0.136(1)	0.027(6)	I
35	0.162(1)	0.019(4)	I
45	0.184(1)	0.028(1)	I
55	0.206(1)	0.033(6)	I
66	0.229(2)	0.049(3)	I
75	0.245(2)	0.068(10)	I
85	0.267(2)	0.240(9)	I
95	0.306(3)	0.646(2)	N
100	0.334(5)	0.801(2)	N
150	0.426(5)	0.917(3)	N
190	0.498(4)	0.953(2)	N
225	0.539(4)	0.916(2)	N
230	0.550(3)	0.962(2)	N
275	0.599(3)	0.947(1)	N
315	0.647(1)	0.979(1)	N
345	0.673(4)	0.980(1)	N
360	0.687(4)	0.983(10)	N
375	0.760(6)	0.686(2)	C_b
385	0.791(6)	0.389(8)	C_b
400	0.827(6)	0.325(7)	C_b
415	0.841(6)	0.328(8)	C_b
450	0.878(6)	0.300(6)	C_b
500	0.903(6)	0.323(1)	C_t
550	0.943(6)	0.337(2)	C_t
600	0.979(6)	0.391(9)	C_t

TABLE XX. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Ts} model described in the main text at $T^* = k_BT/\epsilon_0 = 8.7$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/8.66$.

P^*	η	S_2	Phase/Structure
95	0.191(1)	0.036(1)	I
110	0.207(2)	0.039(8)	I
120	0.218(2)	0.044(6)	I
125	0.222(1)	0.036(8)	I
145	0.244(2)	0.115(2)	I
160	0.267(2)	0.394(7)	I
170	0.285(2)	0.506(1)	I
180	0.312(2)	0.770(3)	N
280	0.429(3)	0.904(7)	N
330	0.474(3)	0.924(3)	N
390	0.520(4)	0.951(2)	N
500	0.593(4)	0.961(2)	N
600	0.650(4)	0.977(9)	N
700	0.700(5)	0.981(1)	N
800	0.747(4)	0.985(5)	N
900	0.846(5)	0.988(5)	C_o
1000	0.905(4)	0.989(6)	C_o
1100	0.950(2)	0.990(5)	C_o

TABLE XXI. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Ts} model described in the main text at $T^* = k_BT/\epsilon_0 = 17.4$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/8.66$.

P^*	η	S_2	Phase/Structure
100	0.137(1)	0.025(7)	I
250	0.226(2)	0.071(2)	I
300	0.260(2)	0.343(1)	I
400	0.350(3)	0.809(9)	N
450	0.380(3)	0.833(6)	N
550	0.436(3)	0.897(5)	N
580	0.450(3)	0.919(3)	N
610	0.464(3)	0.921(3)	N
670	0.491(3)	0.936(3)	N
700	0.503(3)	0.938(2)	N
730	0.516(3)	0.943(3)	N
750	0.524(3)	0.948(2)	N
800	0.543(3)	0.951(3)	N
950	0.595(3)	0.964(1)	N
1000	0.611(3)	0.969(10)	N
1200	0.671(5)	0.973(2)	N
1300	0.698(4)	0.979(9)	N
1400	0.723(5)	0.981(7)	N
1750	0.826(6)	0.987(9)	C_o
1900	0.897(5)	0.988(5)	C_o
2000	0.928(6)	0.989(5)	C_o

TABLE XXII. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Tw} model described in the main text at $T^* = k_BT/\epsilon_0 = 0.875$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/1.76$.

P^*	η	S_2	Phase/Structure
7	0.184(2)	0.040(1)	I
10	0.215(2)	0.025(8)	I
15	0.257(2)	0.063(8)	I
21	0.298(2)	0.217(4)	I
28	0.341(2)	0.254(2)	I
29	0.346(2)	0.210(2)	I
30	0.353(2)	0.258(2)	I
31	0.364(2)	0.162(4)	I
32	0.367(3)	0.202(4)	I
35	0.391(2)	0.088(3)	I
37	0.408(1)	0.083(5)	I
40	0.439(2)	0.143(6)	U
42	0.451(3)	0.185(6)	U
44	0.462(3)	0.127(6)	U
49	0.486(2)	0.198(4)	U
51	0.508(3)	0.099(3)	U
54	0.519(3)	0.133(4)	U
56	0.588(4)	0.394(5)	C_t
60	0.635(5)	0.381(5)	C_t
62	0.622(4)	0.412(6)	C_t
63	0.641(3)	0.402(6)	C_t
65	0.647(3)	0.418(9)	C_t
68	0.651(3)	0.395(8)	C_t
70	0.665(3)	0.387(5)	C_t
83	0.687(3)	0.384(9)	C_t
86	0.693(3)	0.418(4)	C_t
93	0.701(2)	0.412(5)	C_t
100	0.709(2)	0.382(4)	C_t
125	0.733(2)	0.438(3)	C_t
150	0.754(2)	0.435(4)	C_t
200	0.781(2)	0.459(9)	C_t
225	0.793(2)	0.462(4)	C_t
250	0.802(2)	0.489(4)	C_t
300	0.819(2)	0.522(6)	C_t
350	0.833(2)	0.558(4)	C_t
450	0.856(2)	0.580(4)	C_t
600	0.882(1)	0.575(5)	C_t
700	0.896(1)	0.591(6)	C_t
900	0.918(1)	0.633(3)	C_t
1175	0.940(1)	0.589(2)	C_t

TABLE XXIII. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Tw} model described in the main text at $T^* = k_BT/\epsilon_0 = 1.75$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/1.76$.

P^*	η	S_2	Phase/Structure
11	0.147(2)	0.032(1)	I
14	0.165(2)	0.021(9)	I
20	0.195(2)	0.031(8)	I
35	0.254(2)	0.073(3)	I
42	0.279(3)	0.270(3)	I
45	0.288(2)	0.272(3)	I
50	0.302(3)	0.280(4)	I
55	0.321(2)	0.465(3)	N
70	0.362(2)	0.680(2)	N
78	0.380(2)	0.666(1)	N
90	0.407(2)	0.583(8)	N
95	0.416(3)	0.752(10)	N
97	0.425(3)	0.538(7)	N
100	0.427(3)	0.629(2)	N
104	0.435(3)	0.669(1)	N
107	0.447(2)	0.402(1)	N
110	0.448(3)	0.627(9)	N
115	0.472(3)	0.466(1)	N
117	0.471(3)	0.442(9)	N
120	0.482(3)	0.394(1)	N
125	0.494(3)	0.381(2)	N
129	0.506(4)	0.335(2)	N
135	0.551(3)	0.622(7)	C_t
140	0.566(4)	0.608(8)	C_t
145	0.588(3)	0.662(1)	C_t
150	0.596(4)	0.661(8)	C_t
160	0.611(3)	0.675(6)	C_t
180	0.643(3)	0.610(7)	C_t
190	0.655(3)	0.601(1)	C_t
200	0.664(3)	0.640(5)	C_t
240	0.706(3)	0.568(1)	C_t
260	0.718(3)	0.604(4)	C_t
286	0.738(3)	0.579(6)	C_t
300	0.744(3)	0.582(5)	C_t
400	0.790(2)	0.587(6)	C_t
500	0.820(2)	0.642(7)	C_t
700	0.860(2)	0.660(6)	C_t
900	0.888(2)	0.670(4)	C_t
1000	0.899(2)	0.660(5)	C_t
1200	0.919(2)	0.665(3)	C_t
1500	0.941(2)	0.659(5)	C_t

TABLE XXIV. Monte Carlo simulation results for the equation of state and phase behaviour of the U_{Tw} model described in the main text at $T^* = k_BT/\epsilon_0 = 3.5$. The first column correspond to the pressure in reduced units ($P^* = P(L+\sigma)^3/\epsilon_0$). $\eta = \rho\nu_0$ is the packing fraction, with ρ as the particle density and ν_0 as the volume of the particles. S_2 is the nematic order parameter. The values in brackets denote the statistical uncertainty (one standard deviation) in the last digit. The last column indicates the phase corresponding to each state. In this case $P^{**} = P^*/1.76$.

P^*	η	S_2	Phase/Structure
10	0.093(1)	0.017(8)	I
30	0.165(1)	0.021(6)	I
40	0.195(2)	0.388(4)	I
50	0.210(1)	0.040(8)	I
60	0.229(2)	0.053(13)	I
70	0.248(1)	0.065(7)	I
90	0.283(2)	0.200(13)	I
100	0.306(2)	0.564(2)	N
140	0.363(3)	0.732(6)	N
150	0.377(3)	0.774(7)	N
160	0.388(3)	0.804(6)	N
186	0.417(2)	0.841(7)	N
235	0.463(3)	0.803(1)	N
263	0.508(3)	0.811(5)	N
270	0.537(3)	0.873(3)	C_d
280	0.551(4)	0.851(3)	C_d
285	0.560(4)	0.920(3)	C_d
291	0.566(4)	0.932(4)	C_d
310	0.590(3)	0.825(1)	C_d
330	0.604(3)	0.936(2)	C_d
350	0.622(4)	0.879(3)	C_d
380	0.641(4)	0.888(5)	C_d
410	0.660(3)	0.845(5)	C_t
430	0.671(4)	0.888(5)	C_t
450	0.681(3)	0.858(3)	C_t
460	0.686(4)	0.891(5)	C_t
472	0.692(3)	0.871(4)	C_t
500	0.705(4)	0.886(4)	C_t
600	0.742(3)	0.878(2)	C_t
600	0.742(3)	0.882(9)	C_t
700	0.774(3)	0.800(6)	C_t
800	0.799(3)	0.800(4)	C_t
900	0.819(3)	0.782(8)	C_t
1000	0.836(3)	0.836(5)	C_t
1100	0.853(3)	0.776(7)	C_t
1200	0.866(3)	0.826(9)	C_t
1500	0.899(2)	0.753(4)	C_t