

Phase behaviour of mixtures of charged soft disks and spheres

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In this file we collect useful images and informations for all the studied systems. The GB:LJ=1:2 stoichiometry systems are presented first, then the GB:LJ=1:1 and in the end the GB:LJ=2:1 one. For each stoichiometry the different charges are presented from the lower charge ($q_{GB}^*=0.5$) to the higher one ($q_{GB}^*=2.0$).

The document is organized as follows: for each system we report a series of snapshots of the different phases encountered, then the isotropic radial distribution functions, $g(r)$, of the different particle pairs (GB-GB, GB-LJ, LJ-LJ) at some selected temperature to show the close-range order of the Iso, Nem and Col phases; after that we report also the parallel and perpendicular distribution functions, $g(r_{\parallel}^*)$ and $g(r_{\perp}^*)$, for the discotic particle only. In the end the trend of total energy and electrostatic energy are reported as a function of T^* for heating and cooling run. For ordered phases, two snapshots at the same T^* are reported, one showing the top view, that is along the director (left) and the other showing the side view, that is perpendicularly to the director (right). For the isotropic phase only one snapshot is reported. For each serie of snapshot and $g(r)$ the T^* is reported on the left.

The last Figure (Figure S 37) is a summary pressure-temperature diagram for all the studied systems grouped by q_{GB}^* charge.

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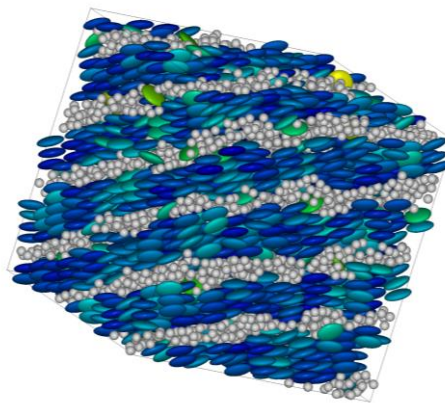
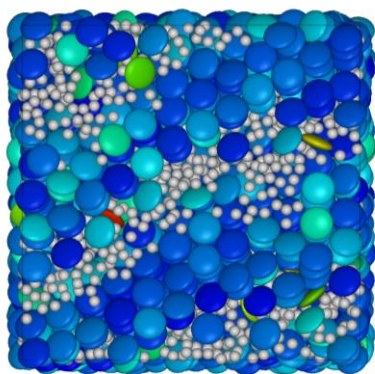
GB:LJ=1:2	$q_{GB}^*=0.5$	$q_{GB}^*=1.0$	$q_{GB}^*=2.0$
Snapshots	Figure S 1	Figure S 5	Figure S 9
$g(r)$	Figure S 2	Figure S 6	Figure S 10
$g(r_{\parallel}^*), g(r_{\perp}^*)$	Figure S 3	Figure S 7	Figure S 11
Energies	Figure S 4	Figure S 8	Figure S 12
GB:LJ=1:1	$q_{GB}^*=0.5$	$q_{GB}^*=1.0$	$q_{GB}^*=2.0$
Snapshots	Figure S 13	Figure S 17	Figure S 21
$g(r)$	Figure S 14	Figure S 18	Figure S 22
$g(r_{\parallel}^*), g(r_{\perp}^*)$	Figure S 15	Figure S 19	Figure S 23
Energies	Figure S 16	Figure S 20	Figure S 24
GB:LJ=2:1	$q_{GB}^*=0.5$	$q_{GB}^*=1.0$	$q_{GB}^*=2.0$
Snapshots	Figure S 25	Figure S 29	Figure S 33
$g(r)$	Figure S 26	Figure S 30	Figure S 34
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Energies	Figure S 28	Figure S 32	Figure S 36

The presented index is linked with the Figures. Click on the Figure's number and the selected Figure will be shown.

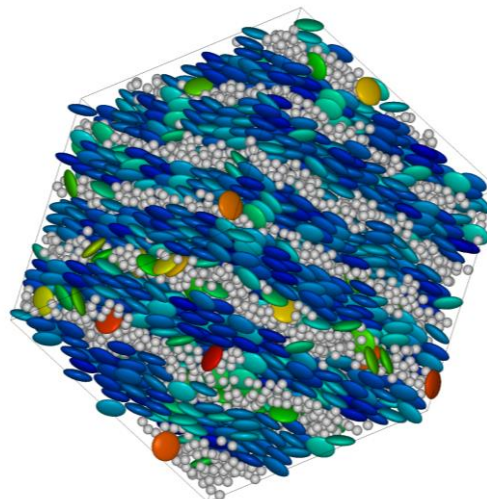
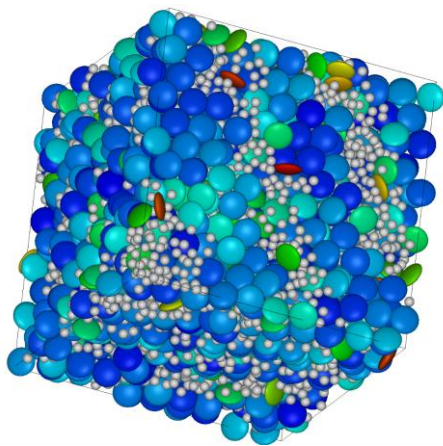
GB:LJ=1:2

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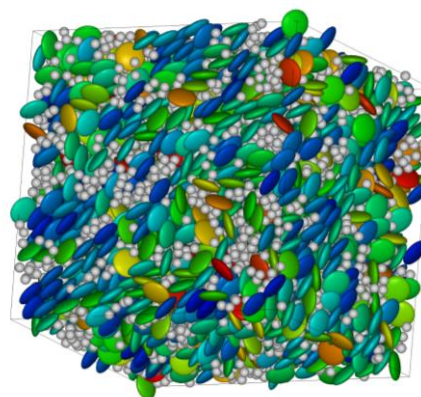
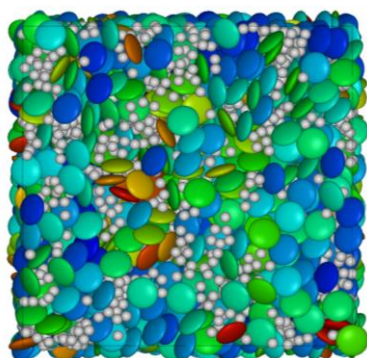
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$T^*=3.00$



$T^*=5.00$



$T^*=8.00$

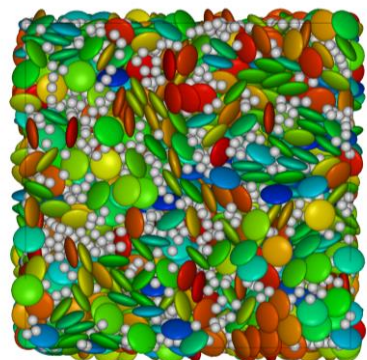


Figure S 1 Snapshots of the GB:LJ=1:2 system, $q_{GB}^*=0.5$ at some selected T^*

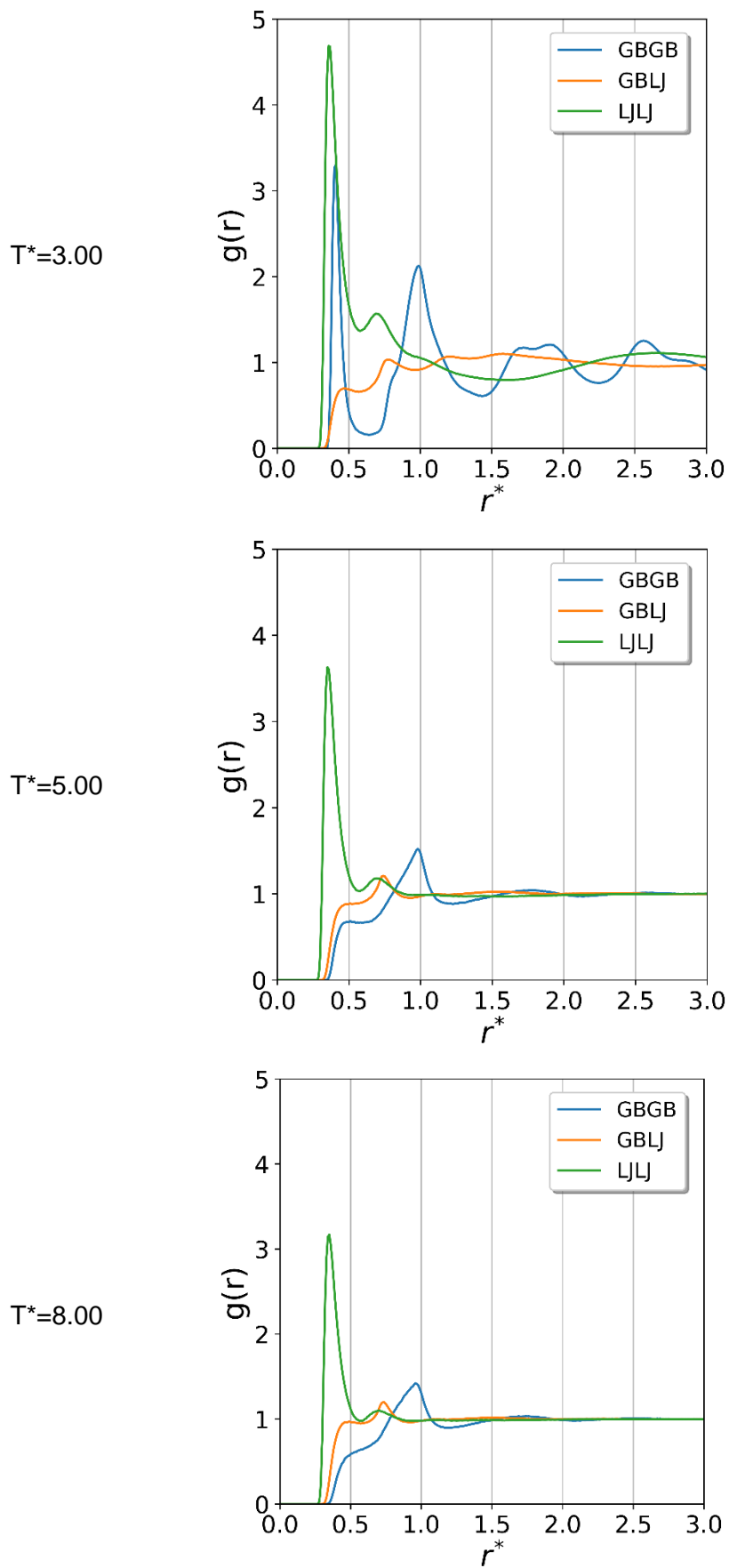


Figure S 2 Radial distribution functions, $g(r)$, of all the particle pairs for the columnar, nematic and isotropic phases, respectively on top, center and bottom

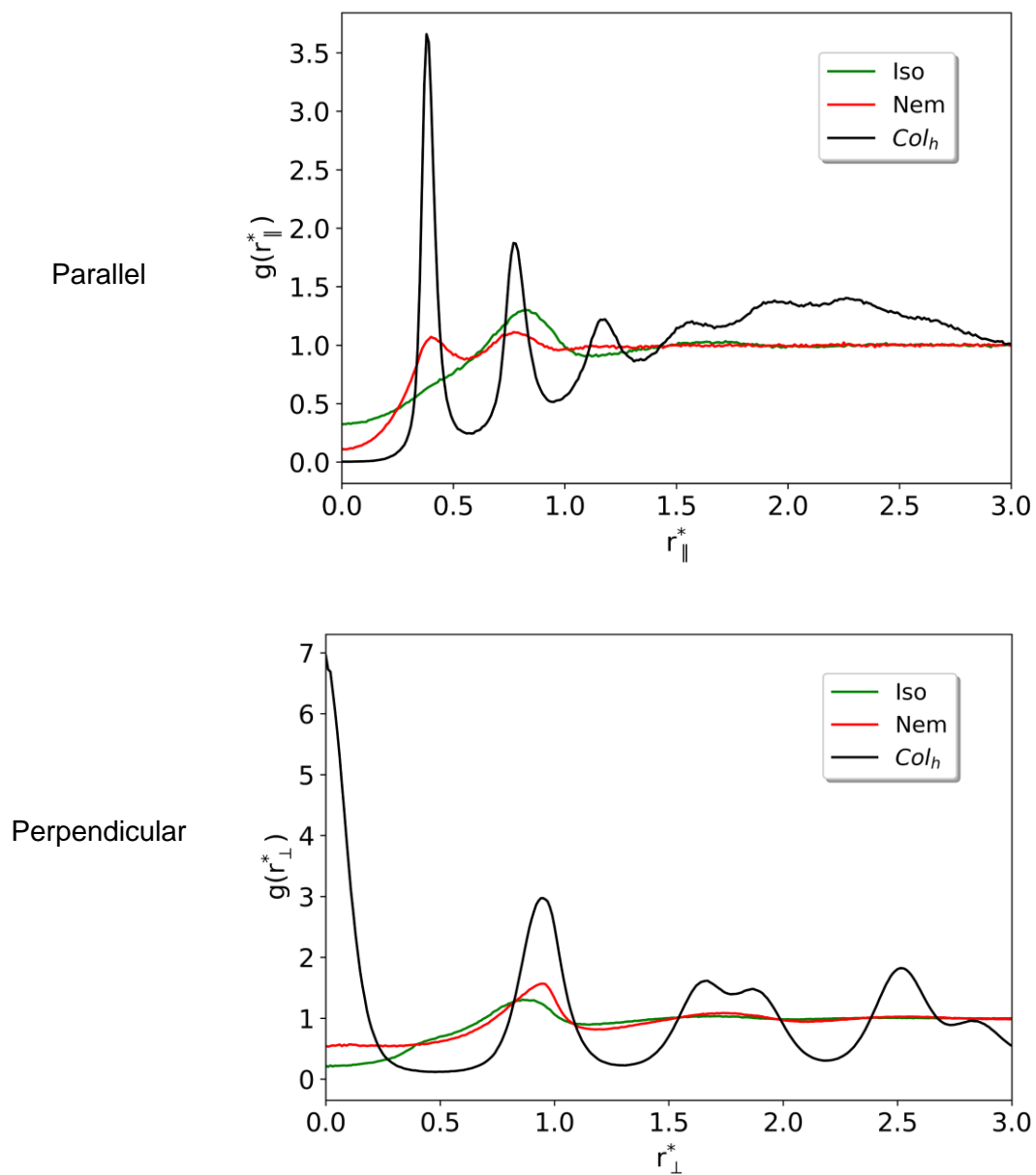


Figure S 3 Parallel, top, and perpendicular, bottom, radial distribution functions, $g(r_{\parallel}^*)$ and $g(r_{\perp}^*)$, of the discotic particles in the columnar (black), nematic (red) and isotropic phases (green). The temperatures of Iso, Nem and Col_h are 8.00, 5.00 and 3.00 respectively

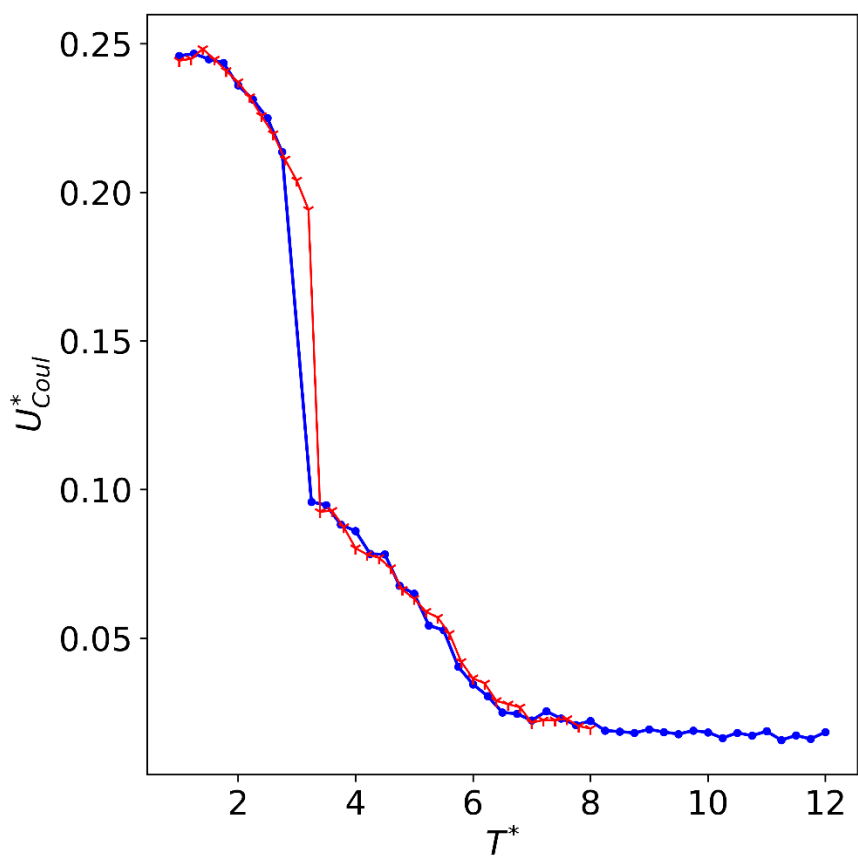
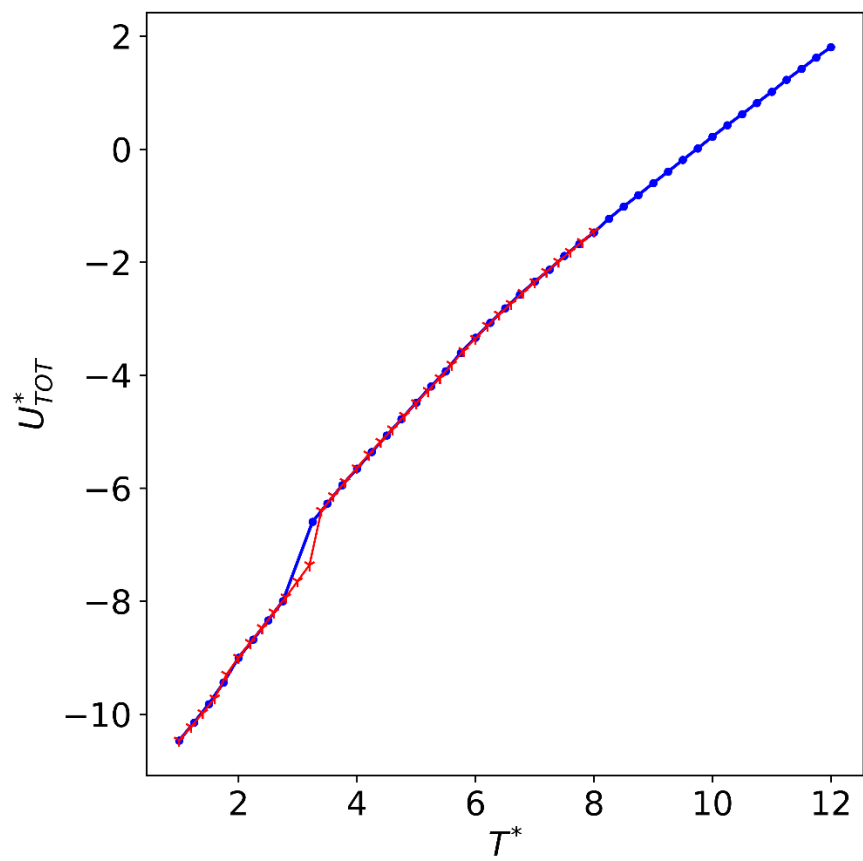
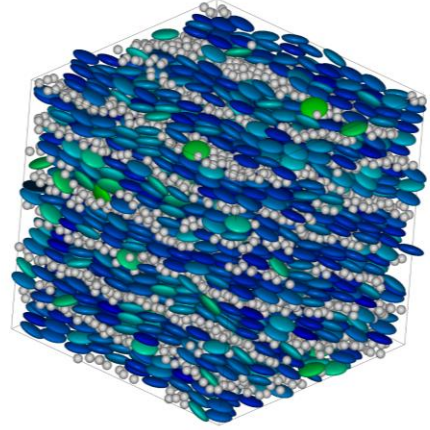
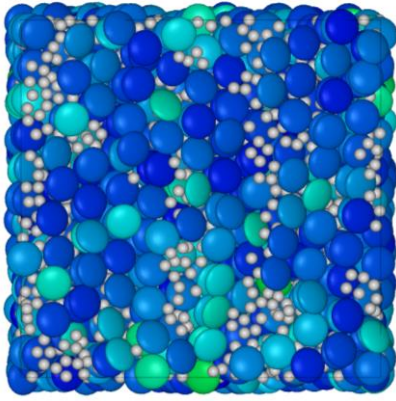


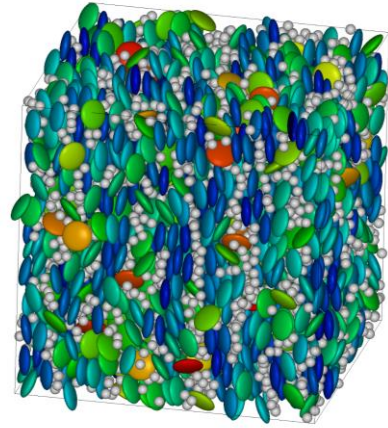
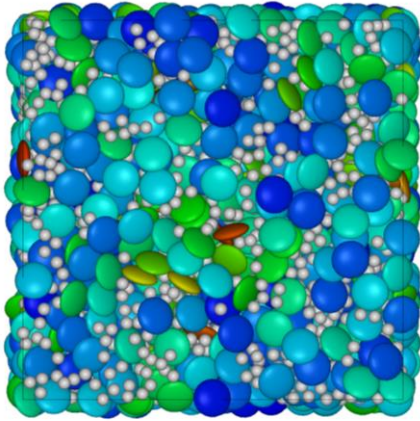
Figure S 4 Total energy (U_{TOT}^*) and electrostatic energy (U_{Coul}^*) as a function of temperature for the GB:LJ=1:2 and $q_{GB}^*=0.5$ system. Heating runs are represented in red, while cooling runs are represented in blue

$$q_{GB}^* = 1.00$$

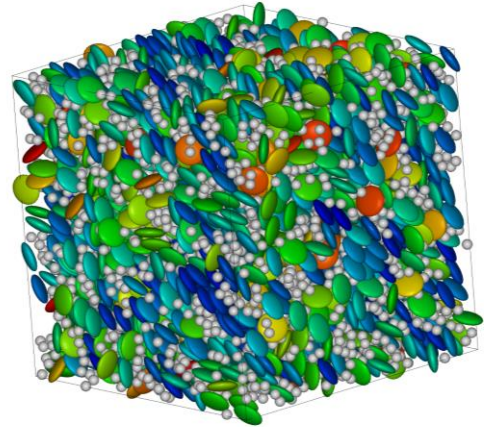
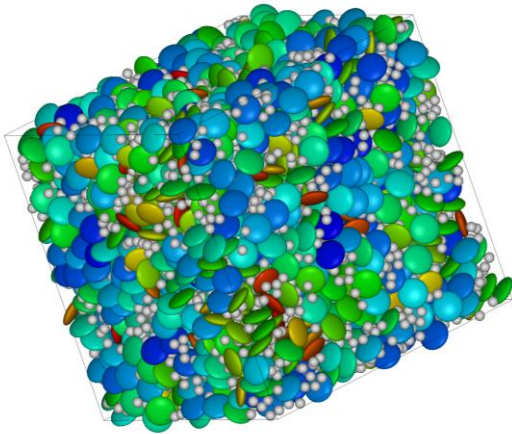
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$T^*=3.00$



$T^*=4.00$



$T^*=6.00$

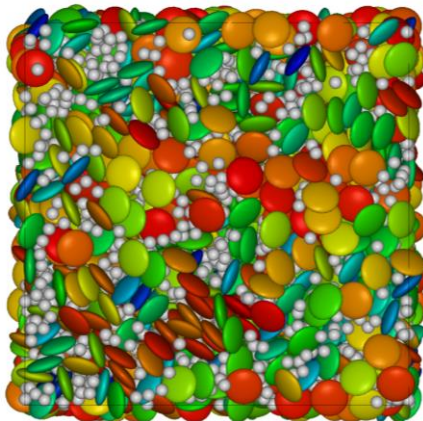


Figure S 5 Snapshots of the GB:LJ=1:2 system, $q_{GB}^*=1.0$ at some selected T^*

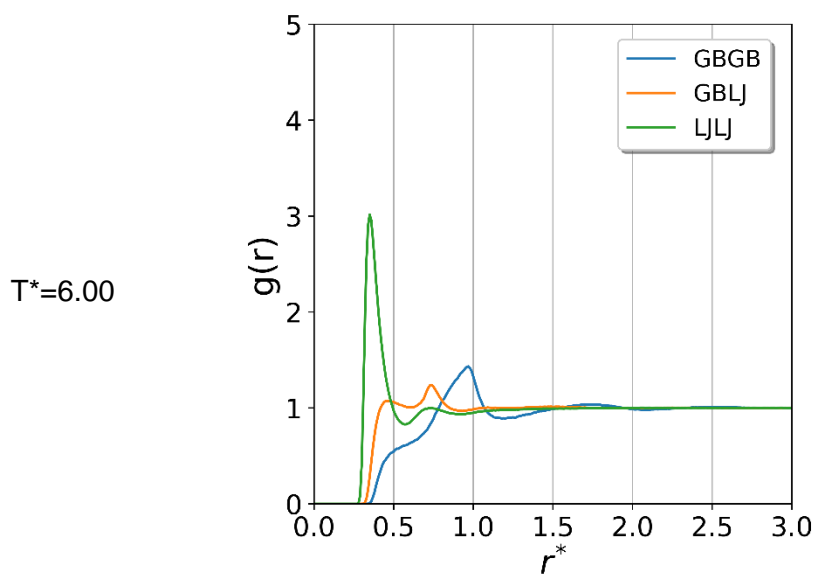
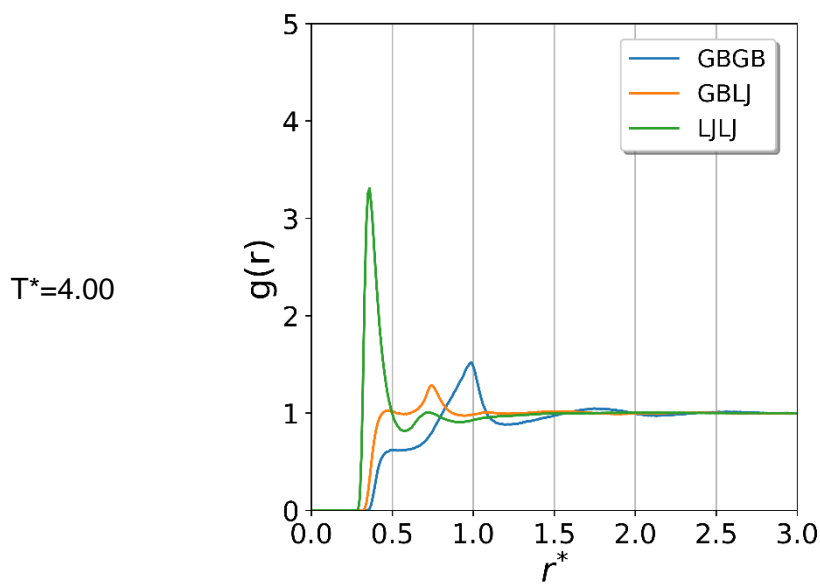
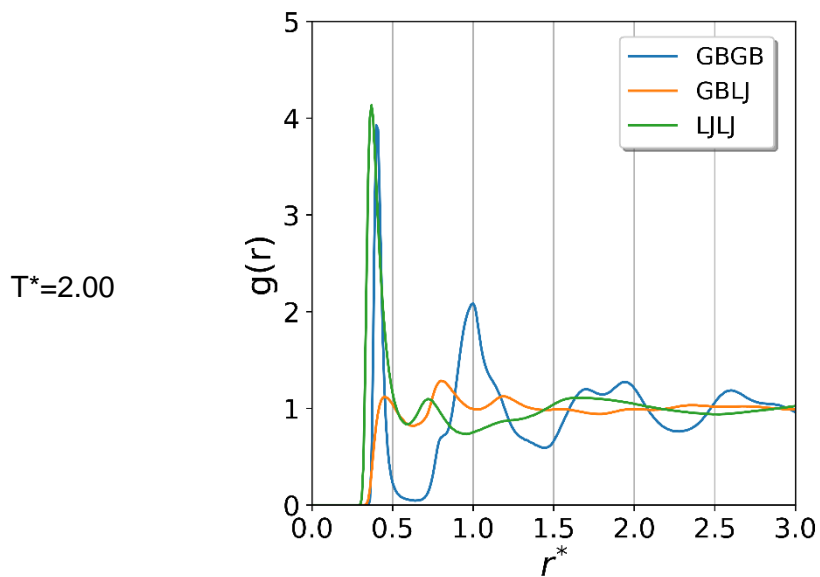


Figure S 6 Radial distribution functions, $g(r)$, of all the particle pairs for the columnar, nematic and isotropic phases, respectively on top, center and bottom

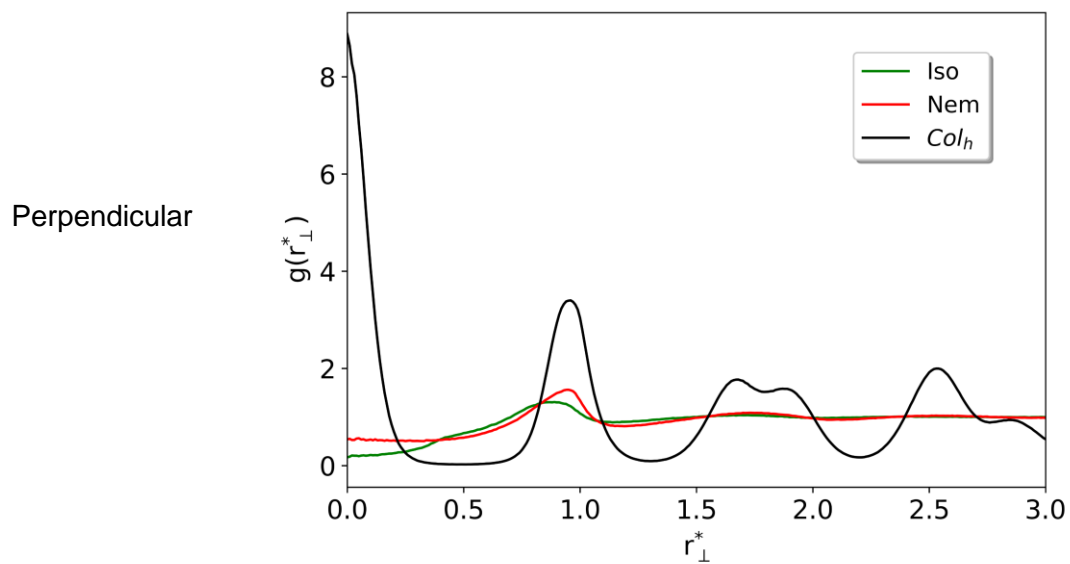
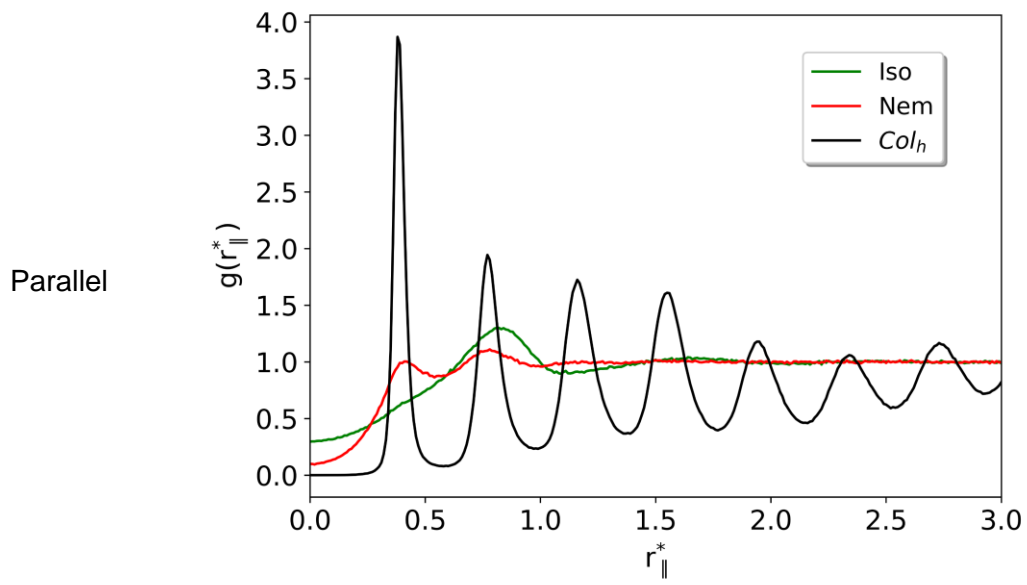


Figure S 7 Parallel, top, and perpendicular, bottom, radial distribution functions, $g(r_{\parallel}^*)$ and $g(r_{\perp}^*)$, of the discotic particles in the columnar (black), nematic (red) and isotropic phases (green). The temperatures of Iso, Nem and Col_h are 6.00, 4.00 and 2.00 respectively

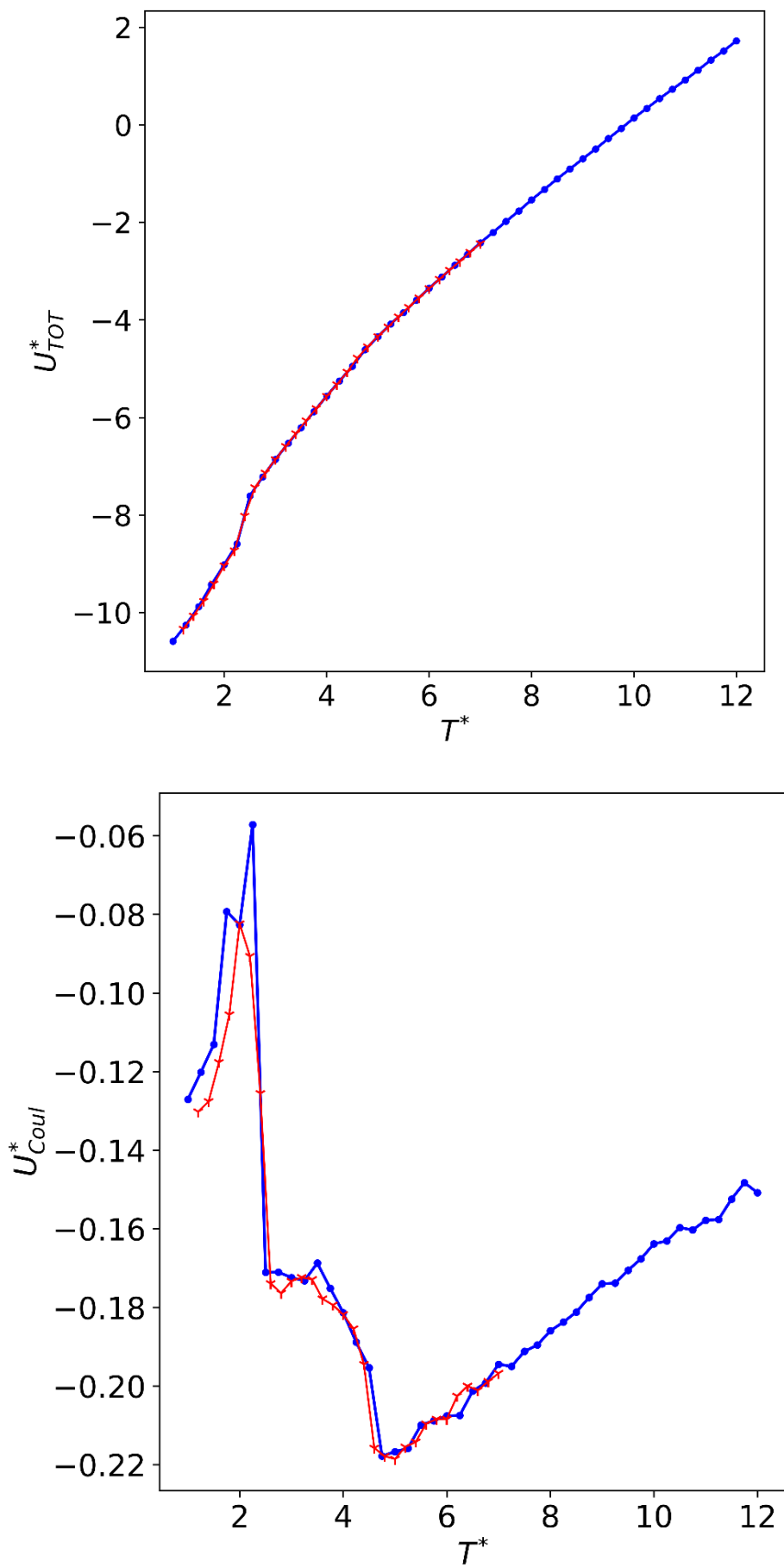
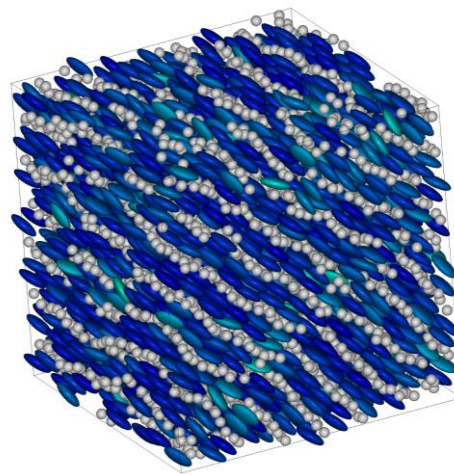
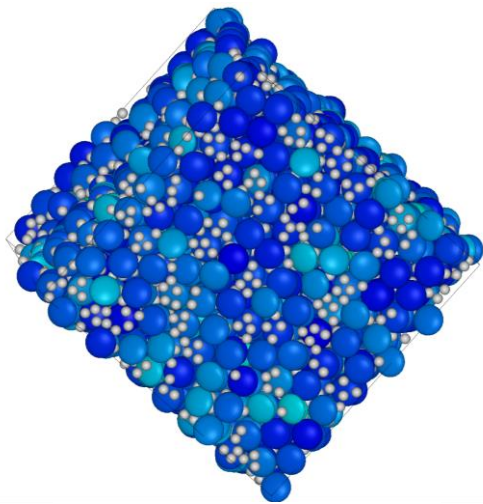


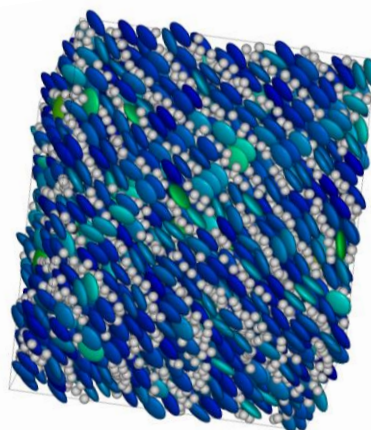
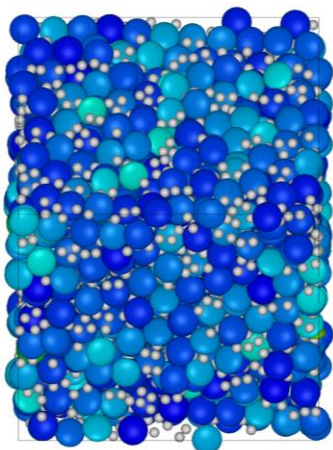
Figure S 8 Total energy (U_{TOT}^*) and electrostatic energy (U_{Coul}^*) as a function of temperature for the GB:LJ=1:2 and $q_{GB}^*=1.0$ system. Heating runs are represented in red, while cooling runs are represented in blue

$$q_{GB}^* = 2.00$$

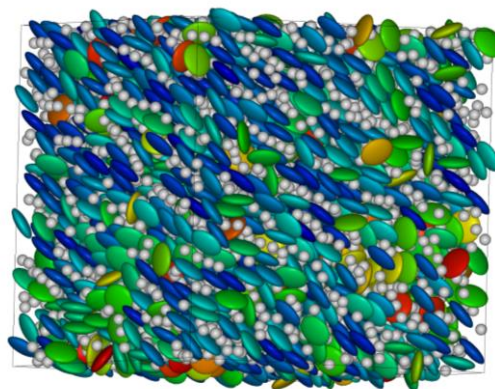
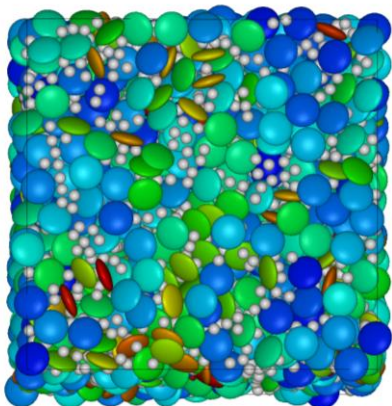
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$T^*=1.30$



$T^*=1.70$



$T^*=2.30$

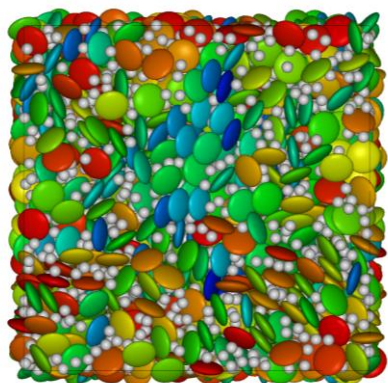


Figure S 9 Snapshots of the GB:LJ=1:2 system, $q_{GB}^*=2.0$ at some selected T^*

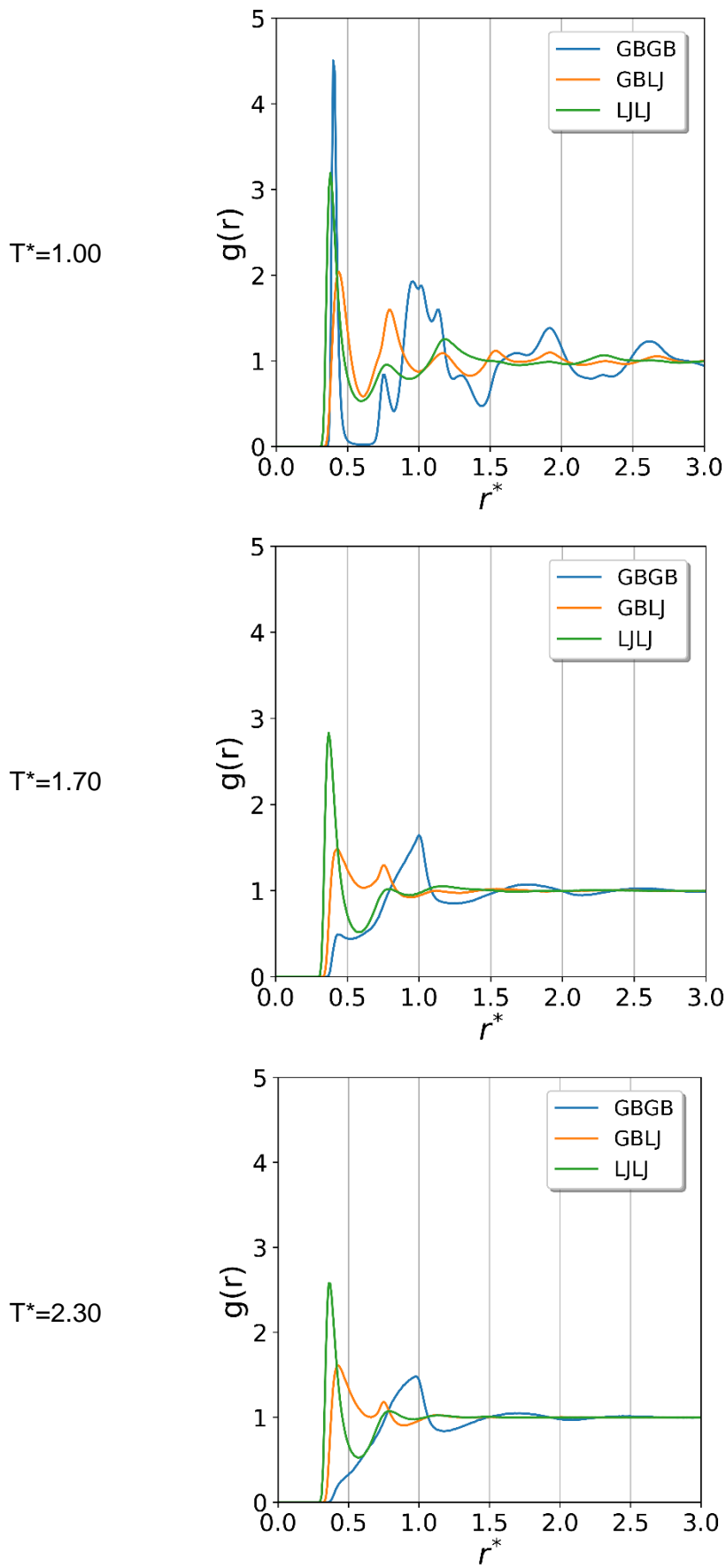


Figure S 10 Radial distribution functions, $g(r)$, of all the particle pairs for the columnar, nematic and isotropic phases, respectively on top, center and bottom

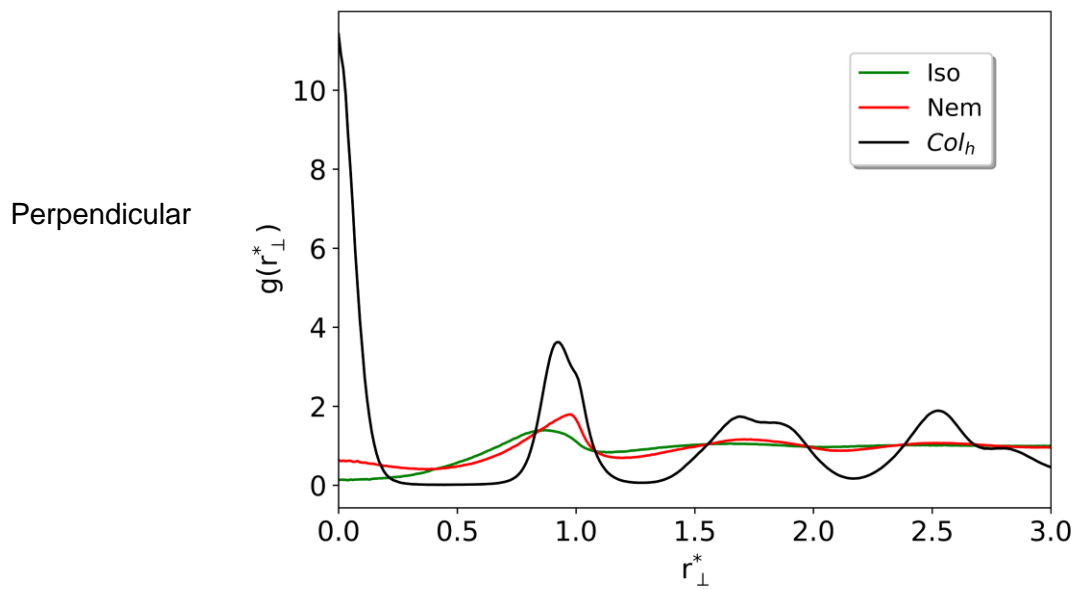
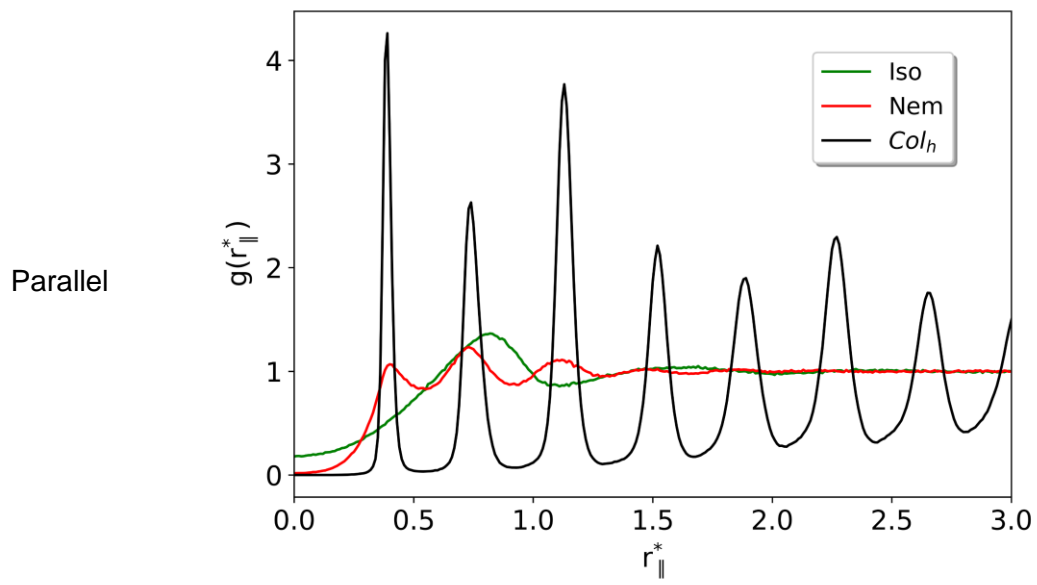


Figure S 11 Parallel, top, and perpendicular, bottom, radial distribution functions, $g(r_{\parallel}^*)$ and $g(r_{\perp}^*)$, of the discotic particles in the columnar (black), nematic (red) and isotropic phases (green). The temperatures of Iso, Nem and Col_h are 2.30, 1.70 and 1.00 respectively

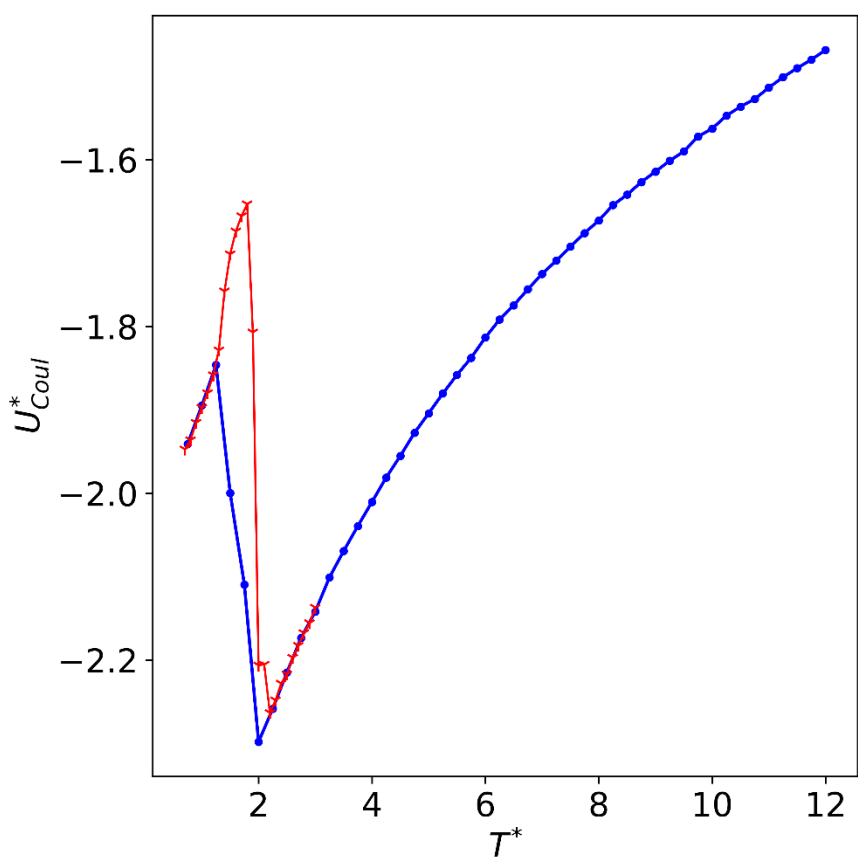
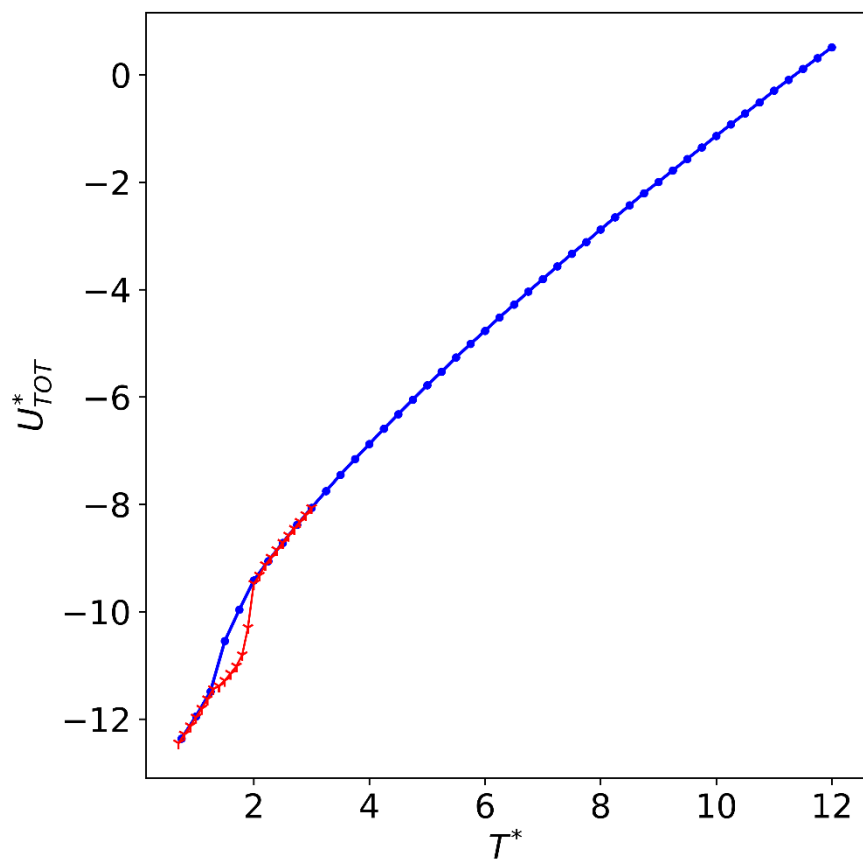
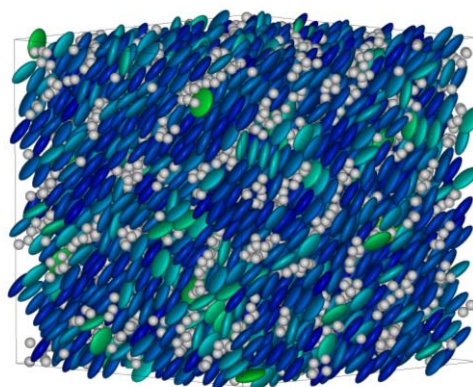
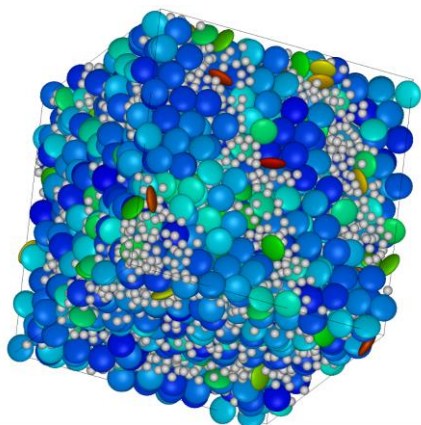


Figure S 12 Total energy (U_{TOT}^*) and electrostatic energy (U_{Coul}^*) as a function of temperature for the GB:LJ=1:2 and $q_{GB}^*=2.0$ system. Heating runs are represented in red, while cooling runs are represented in blue

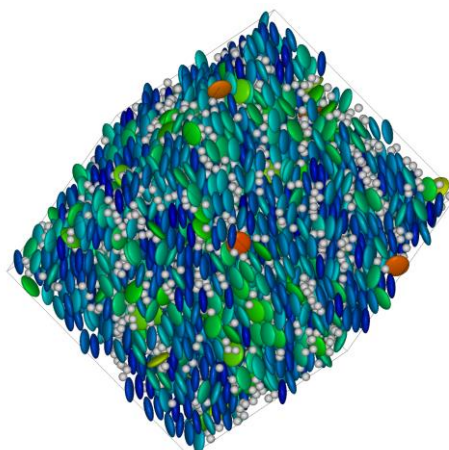
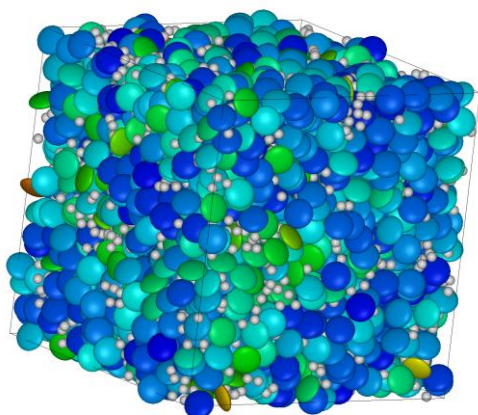
GB:LJ=1:1

$$q_{GB}^* = 0.50$$

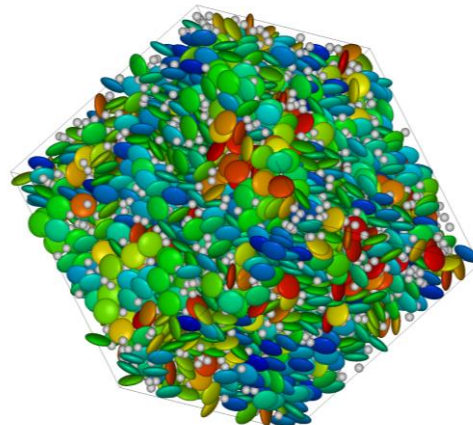
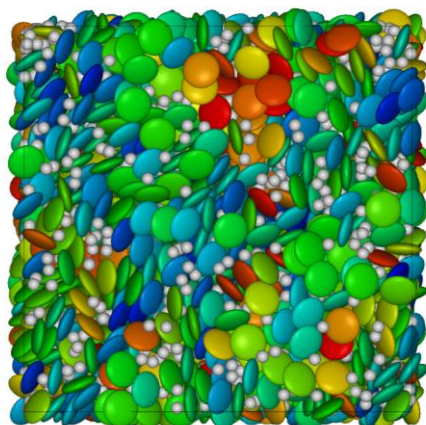
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$T^*=3.00$



$T^*=7.00$



$T^*=9.00$

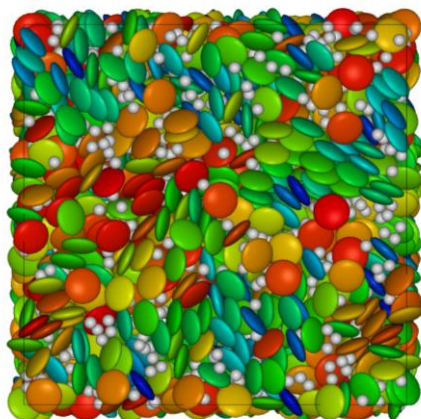


Figure S 13 Snapshots of the GB:LJ=1:1 system, $q_{GB}^*=0.5$ at some selected T^*

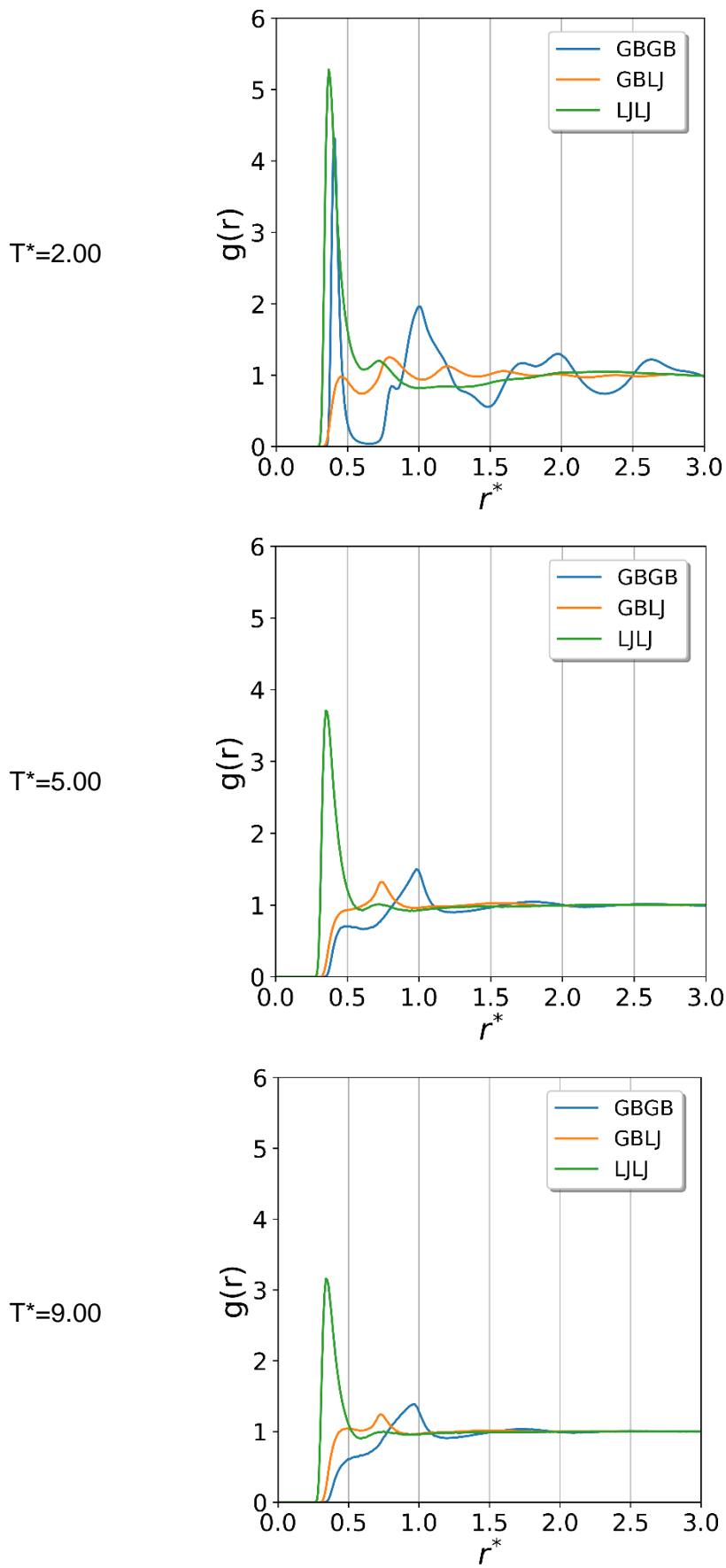


Figure S 14 Radial distribution functions, $g(r)$, of all the particle pairs for the columnar, nematic and isotropic phases, respectively on top, center and bottom

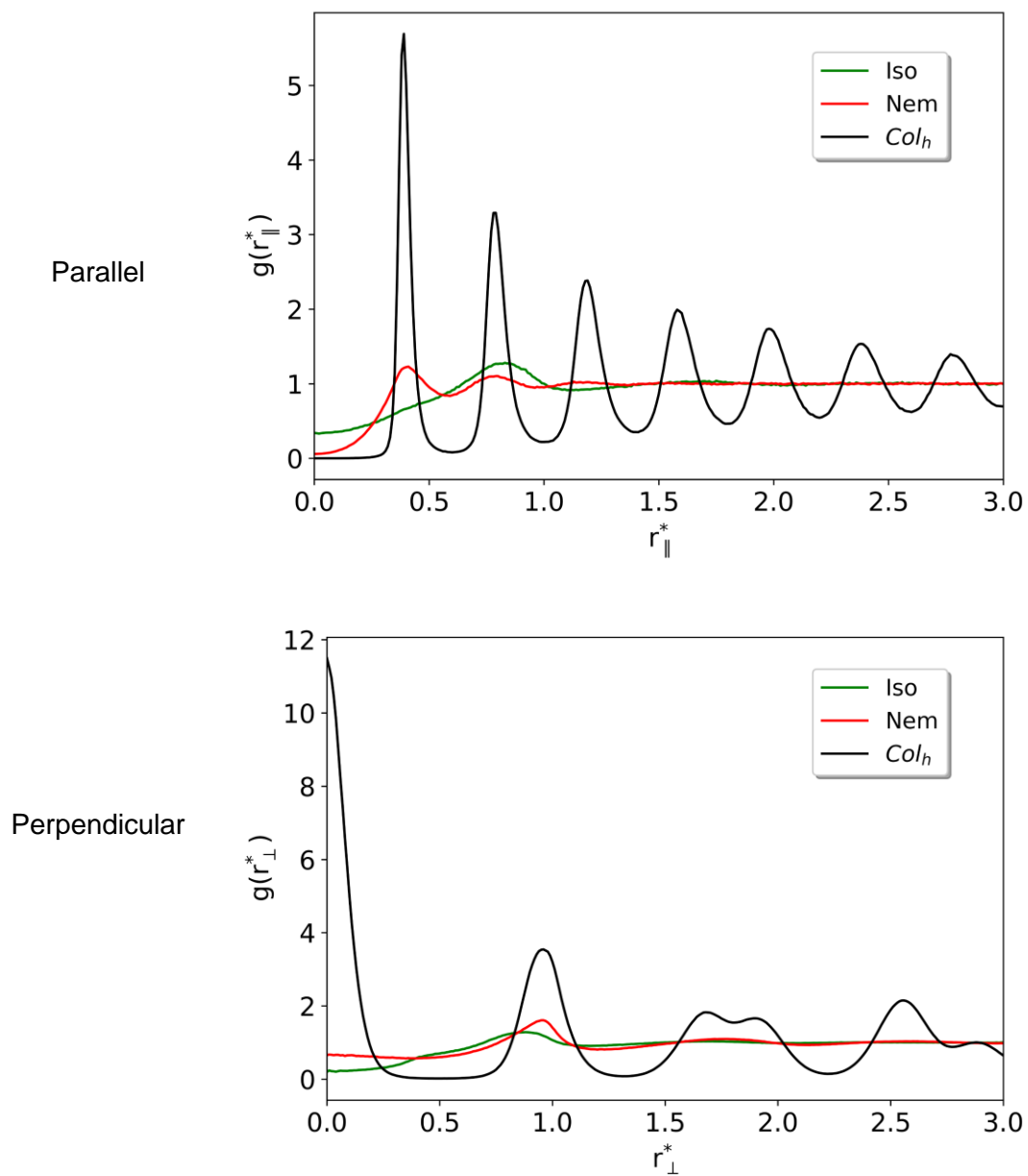


Figure S 15 Parallel, top, and perpendicular, bottom, radial distribution functions, $g(r_{\parallel}^*)$ and $g(r_{\perp}^*)$, of the discotic particles in the columnar (black), nematic (red) and isotropic phases (green). The temperatures of Iso, Nem and Col_h are 9.00, 5.00 and 2.00 respectively

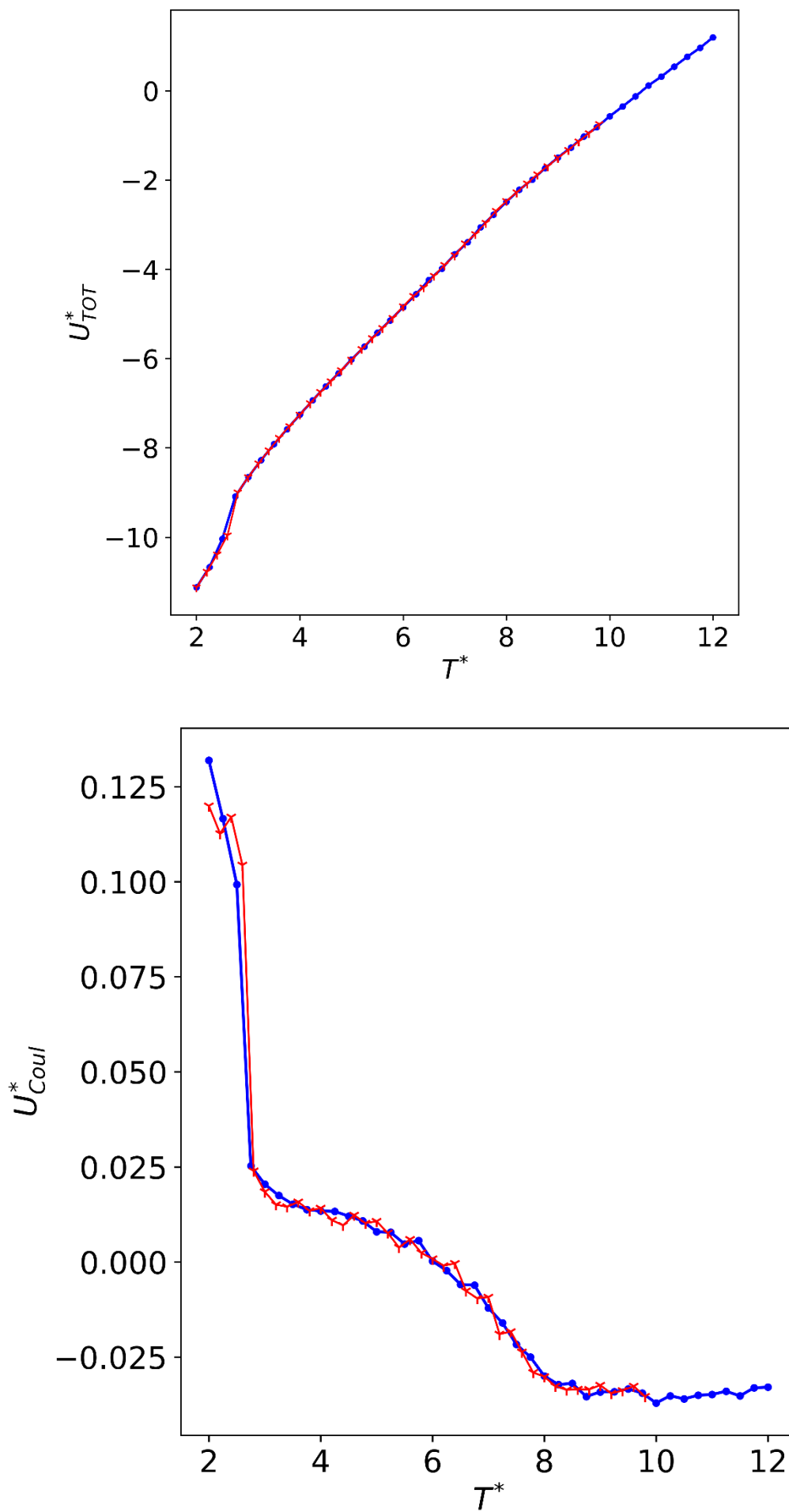
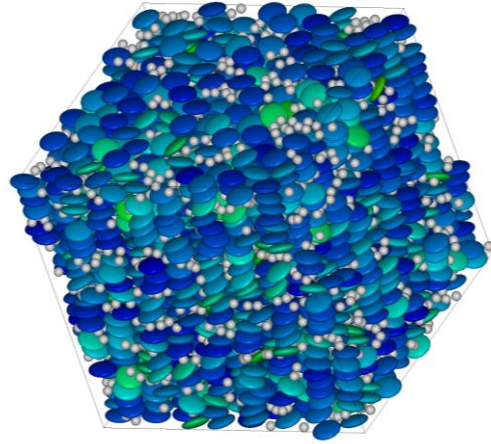
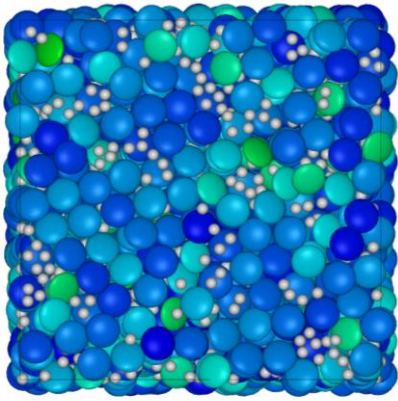


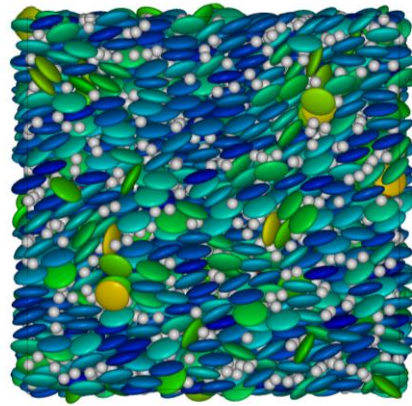
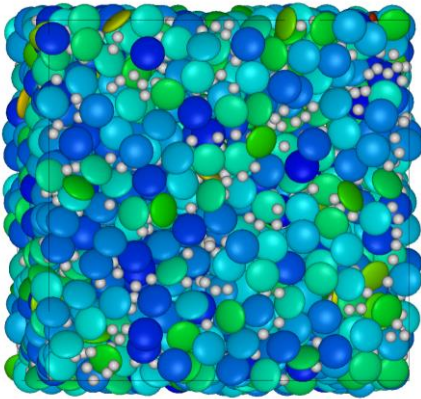
Figure S 16 Total energy (U_{TOT}^*) and electrostatic energy (U_{Coul}^*) as a function of temperature for the GB:LJ=1:1 and $q_{GB}^*=0.5$ system. Heating runs are represented in red, while cooling runs are represented in blue

$$q_{GB}^* = 1.00$$

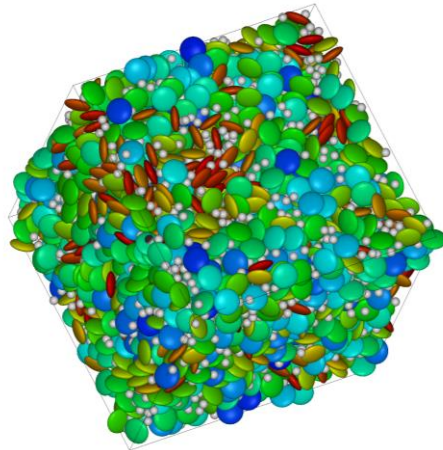
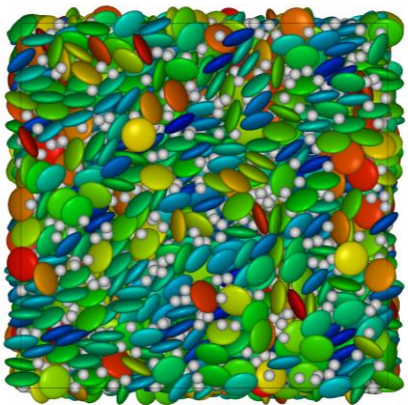
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$T^*=3.00$



$T^*=6.00$



$T^*=8.00$

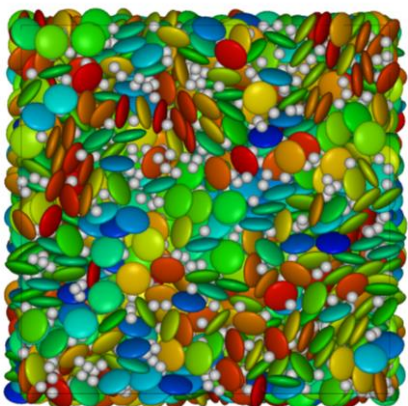


Figure S 17 Snapshots of the GB:LJ=1:1 system, $q_{GB}^*=1.0$ at some selected T^*

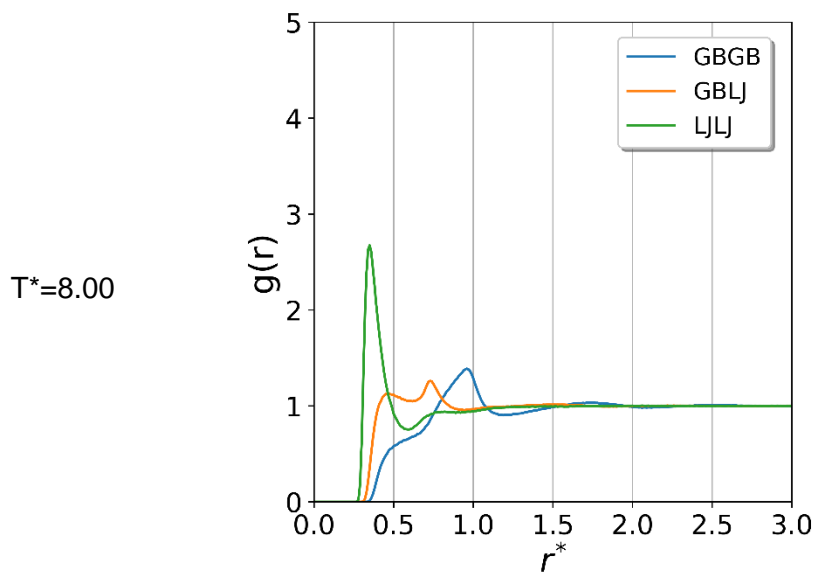
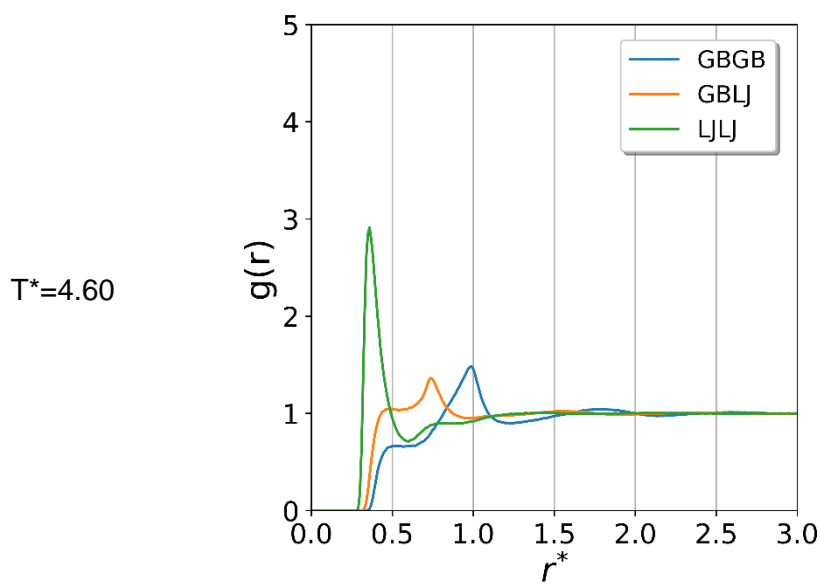
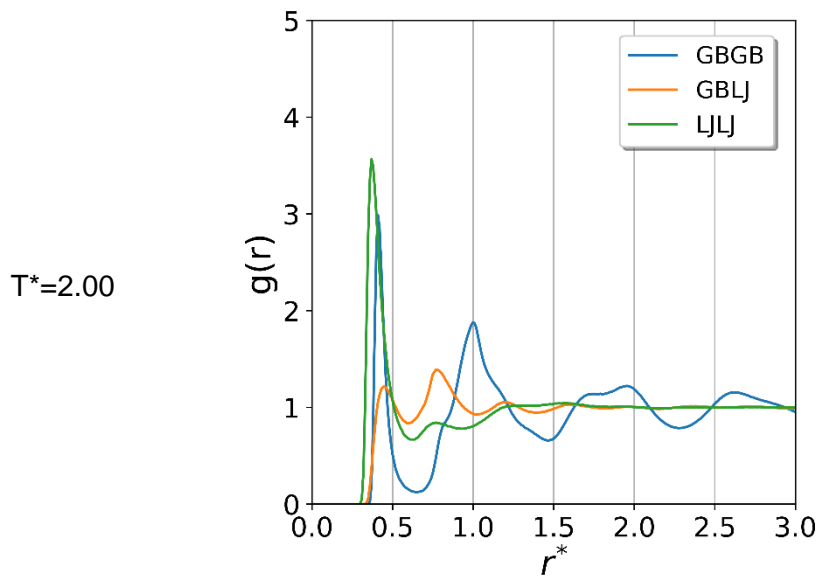


Figure S 18 Radial distribution functions, $g(r)$, of all the particle pairs for the columnar, nematic and isotropic phases, respectively on top, center and bottom

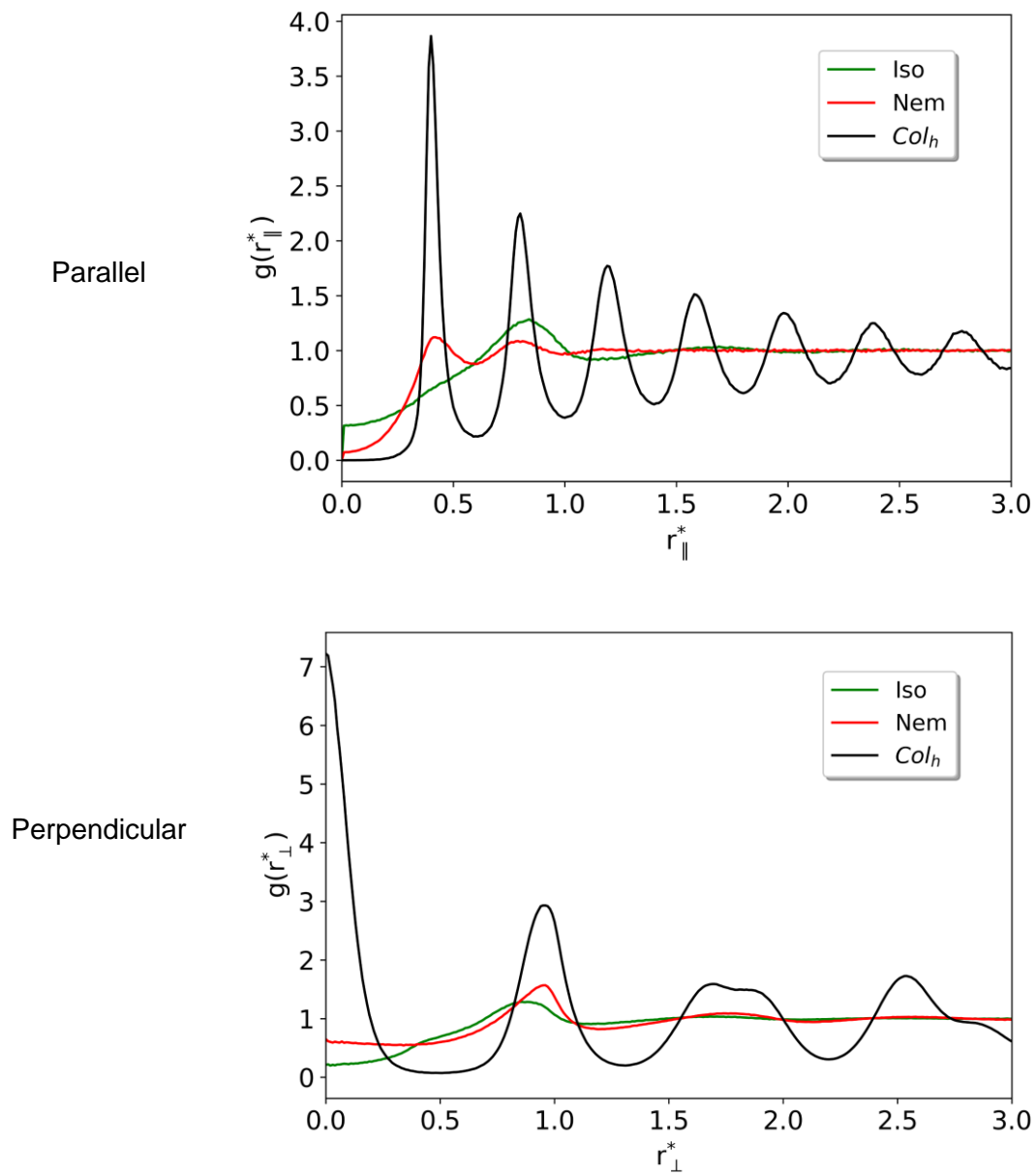


Figure S 19 Parallel, top, and perpendicular, bottom, radial distribution functions, $g(r_{\parallel}^*)$ and $g(r_{\perp}^*)$, of the discotic particles in the columnar (black), nematic (red) and isotropic phases (green). The temperatures of Iso, Nem and Col_h are 8.00, 4.60 and 2.00 respectively

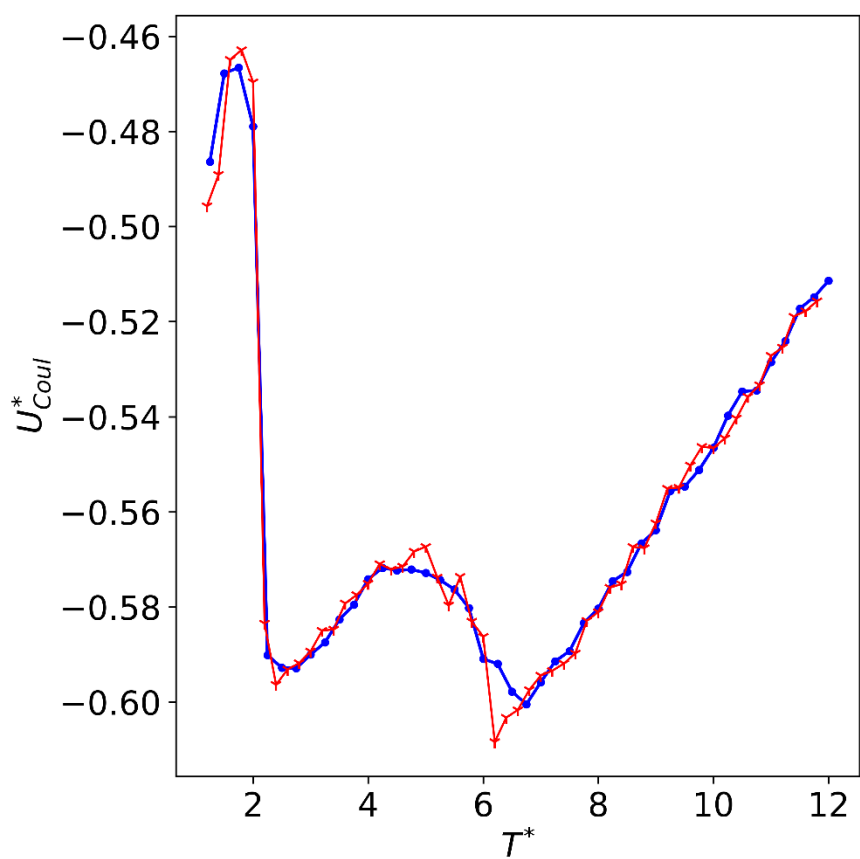
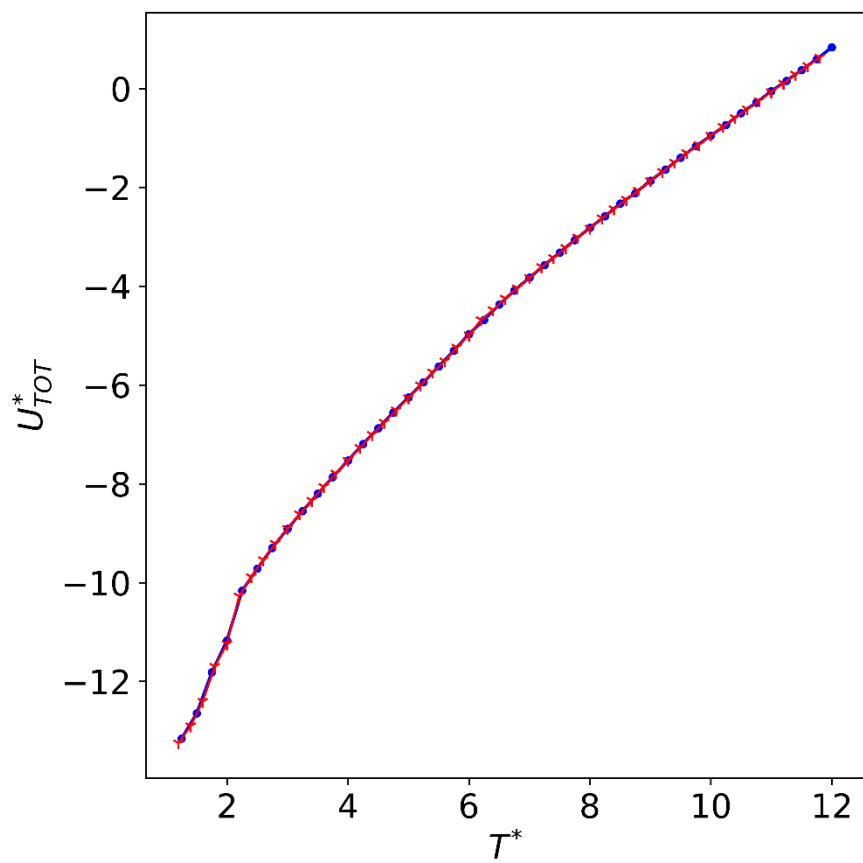
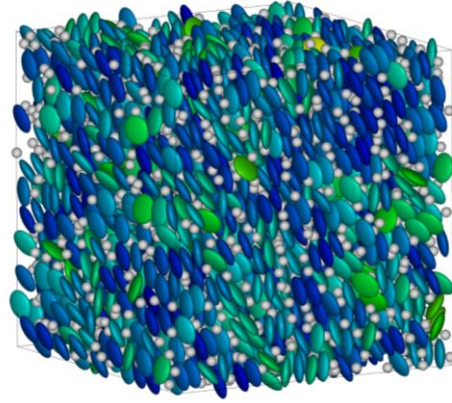
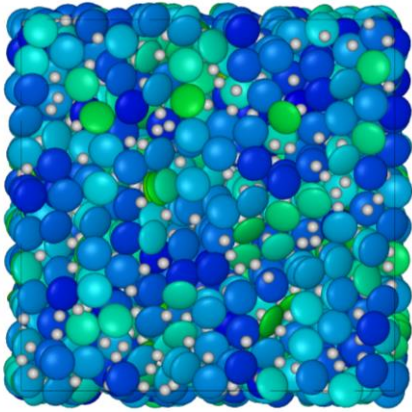


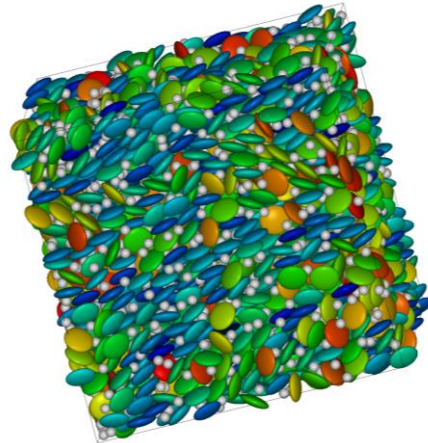
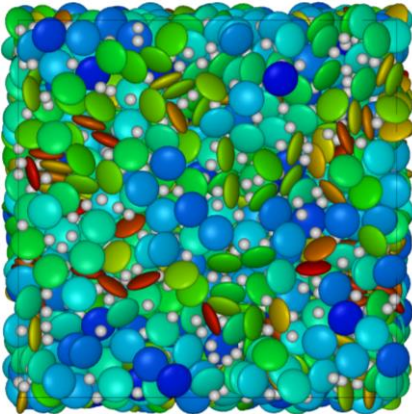
Figure S 20 Total energy (U_{TOT}^*) and electrostatic energy (U_{Coul}^*) as a function of temperature for the GB:LJ=1:1 and $q_{GB}^*=1.0$ system. Heating runs are represented in red, while cooling runs are represented in blue

$$q_{GB}^* = 2.00$$

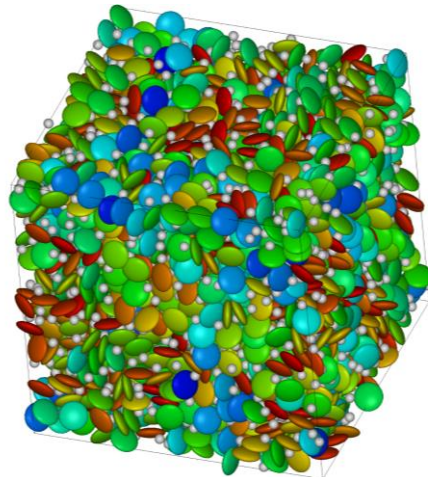
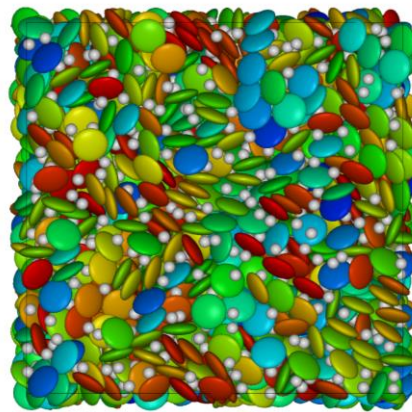
$T^*=1.00$



$T^*=1.70$



$T^*=2.00$



$T^*=2.30$

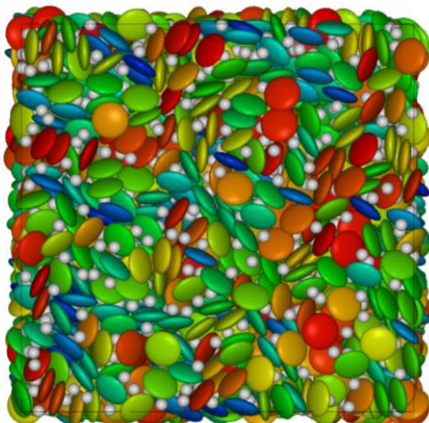


Figure S 21 Snapshots of the GB:LJ=1:1 system, $q_{GB}^*=2.0$ at some selected T^*

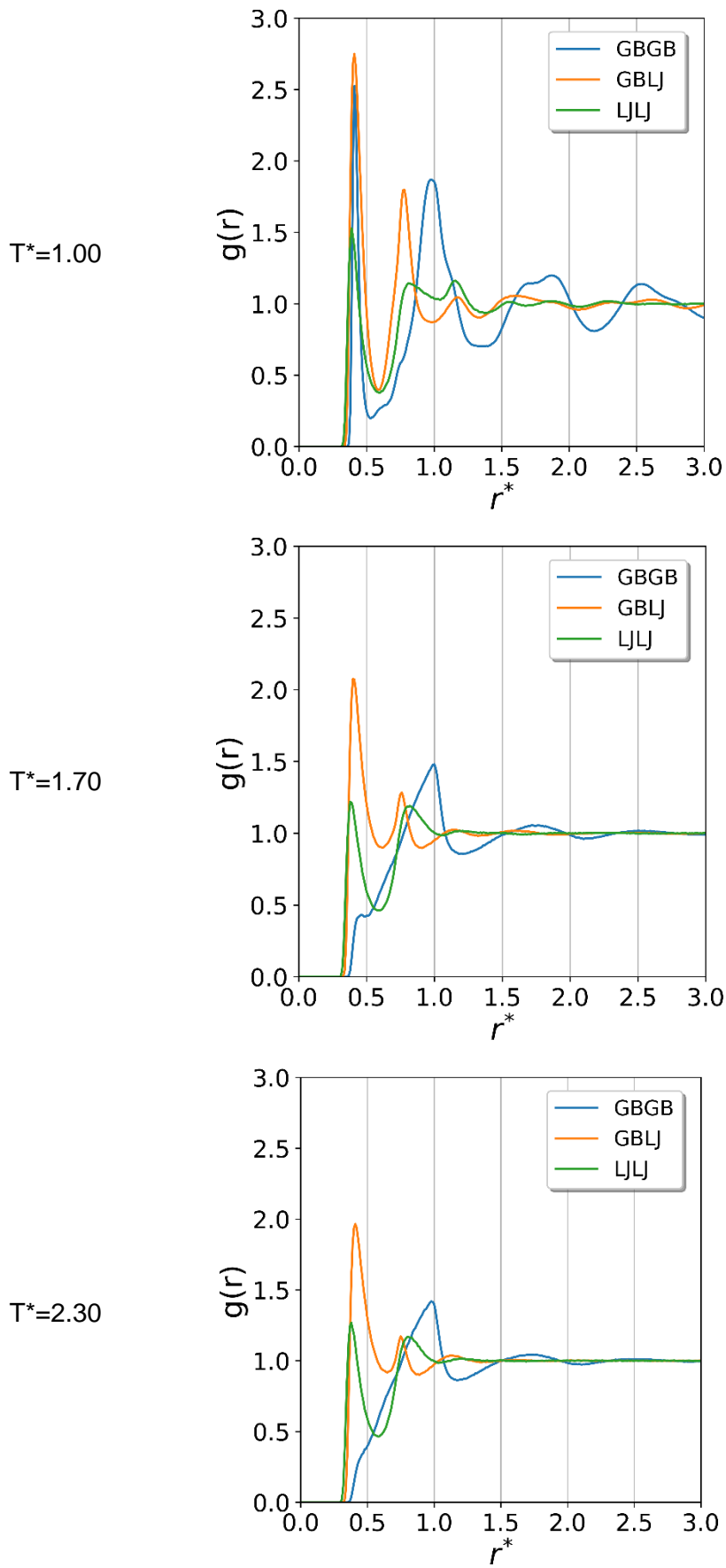


Figure S 22 Radial distribution functions, $g(r)$, of all the particle pairs for the columnar, nematic and isotropic phases, respectively on top, center and bottom

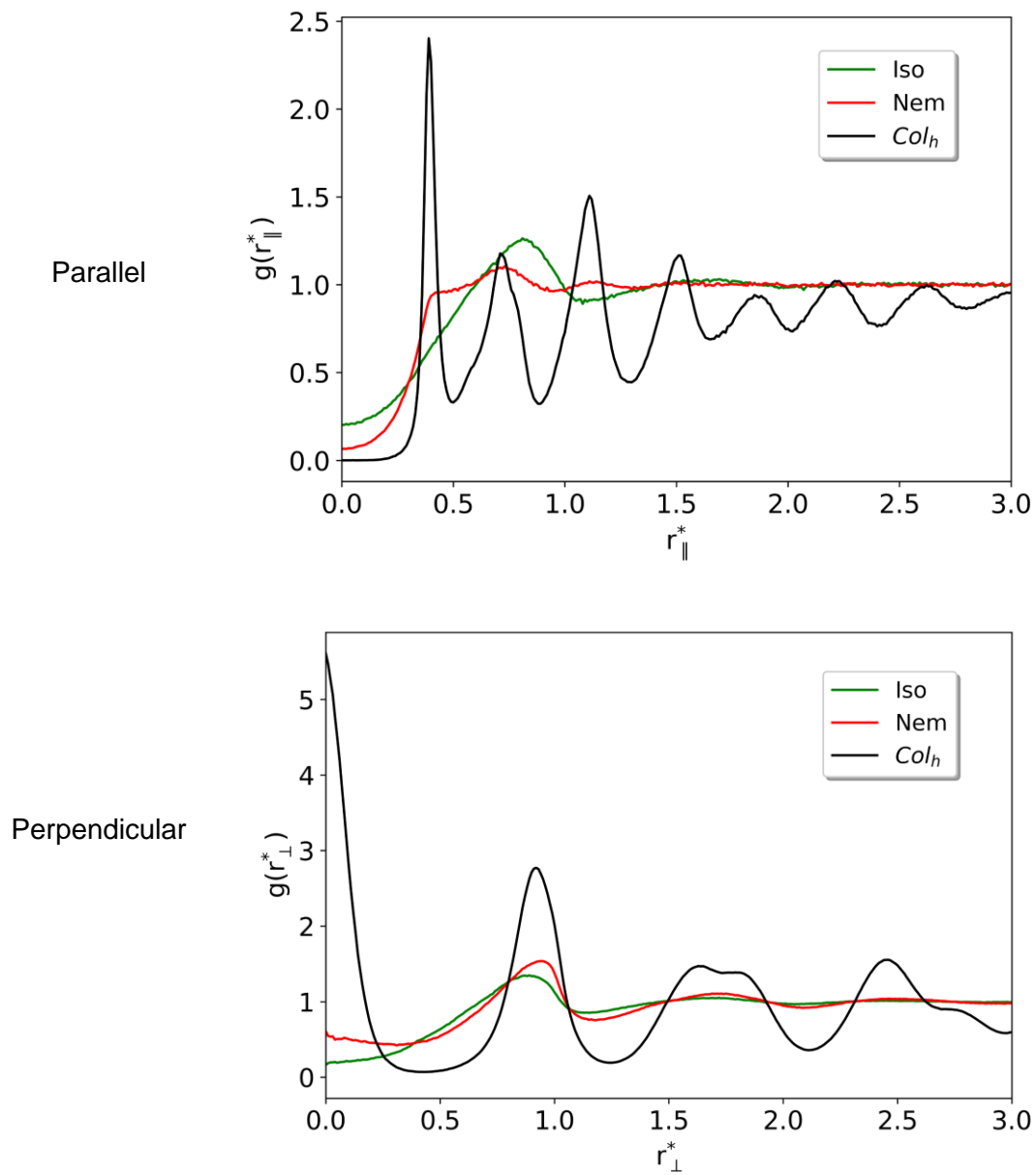


Figure S 23 Parallel, top, and perpendicular, bottom, radial distribution functions, $g(r_{\parallel}^*)$ and $g(r_{\perp}^*)$, of the discotic particles in the columnar (black), nematic (red) and isotropic phases (green). The temperatures of Iso, Nem and Col_h are 2.30, 1.70 and 1.00 respectively

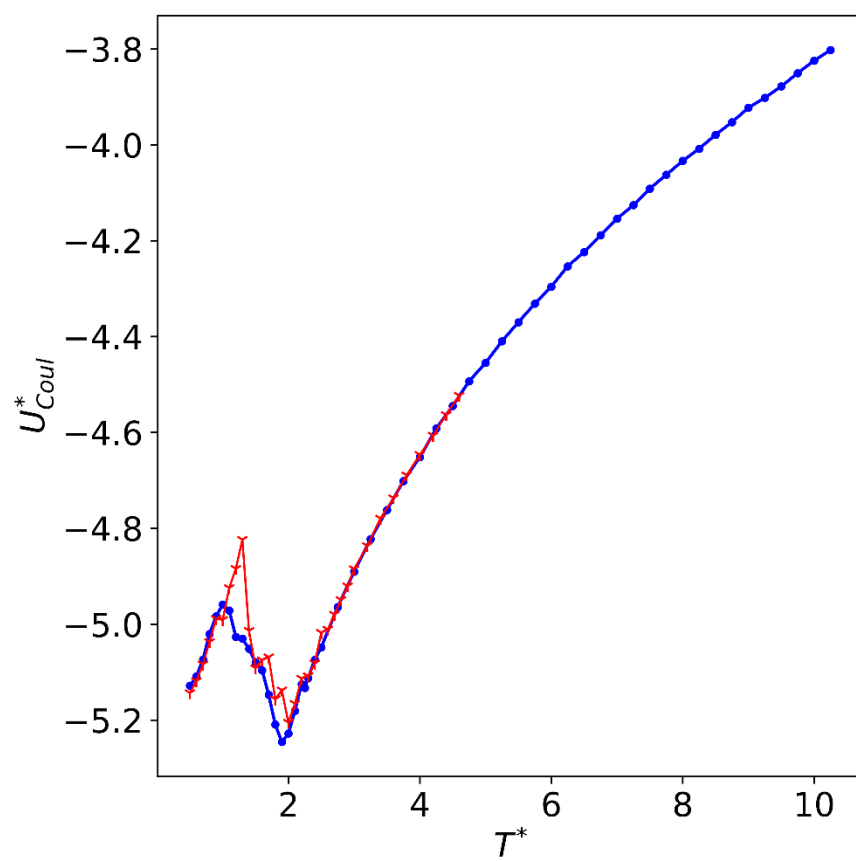
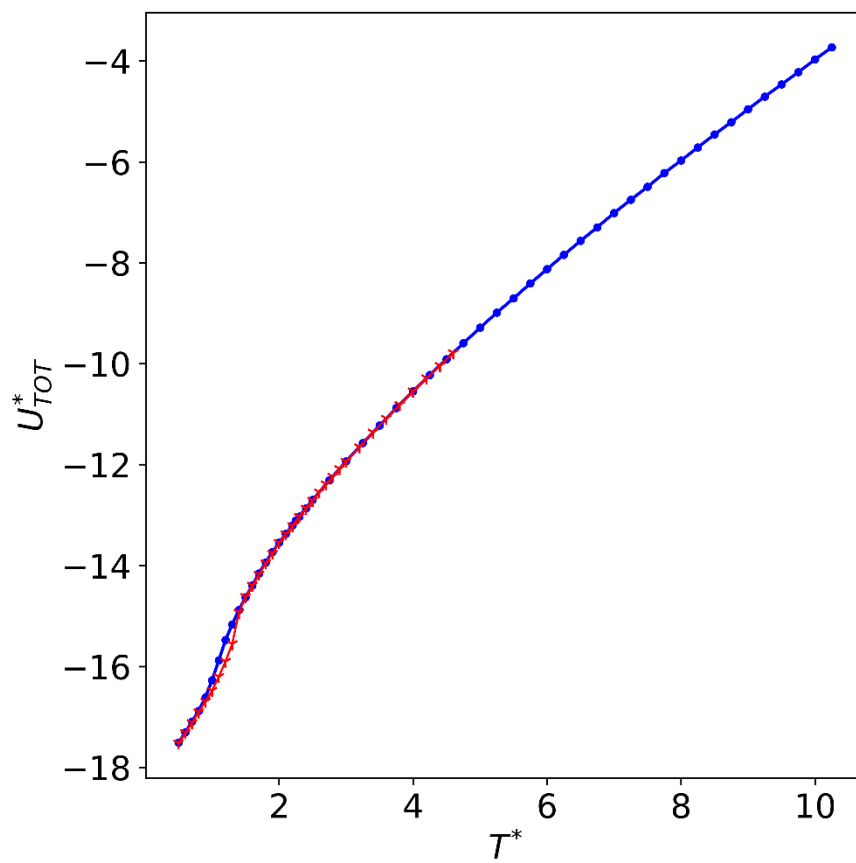
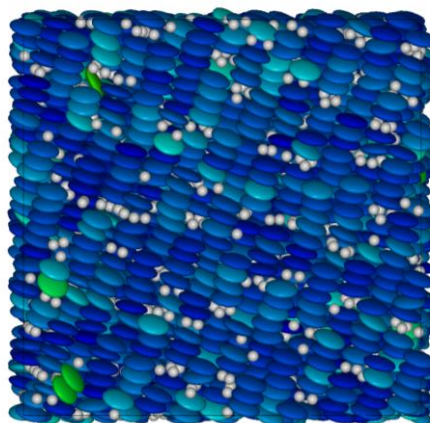
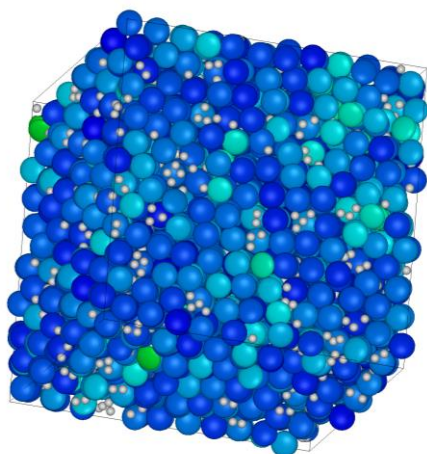


Figure S 24 Total energy (U_{TOT}^*) and electrostatic energy (U_{Coul}^*) as a function of temperature for the GB:LJ=1:1 and $q_{GB}^*=2.0$ system. Heating runs are represented in red, while cooling runs are represented in blue

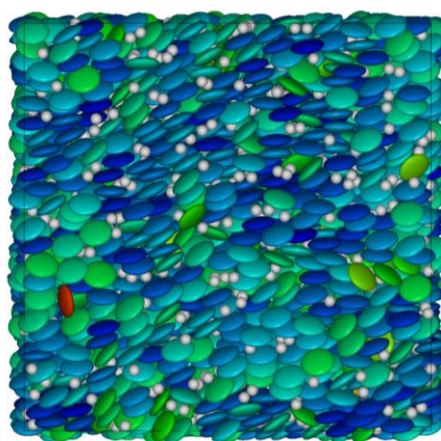
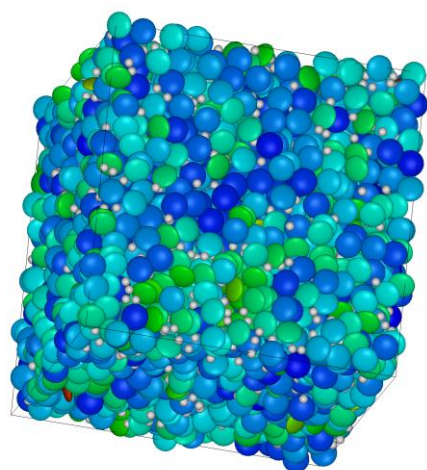
GB:LJ=2:1

$$q_{GB}^* = 0.50$$

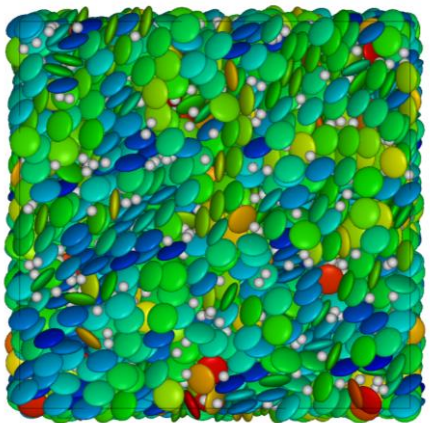
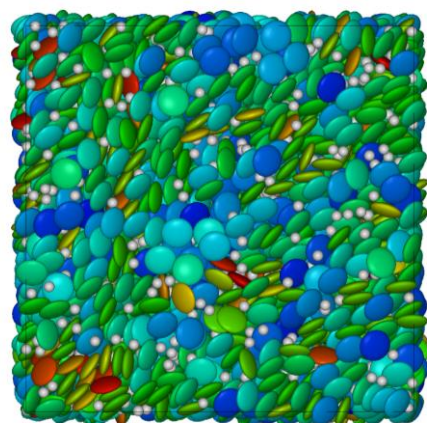
$T^*=1.50$



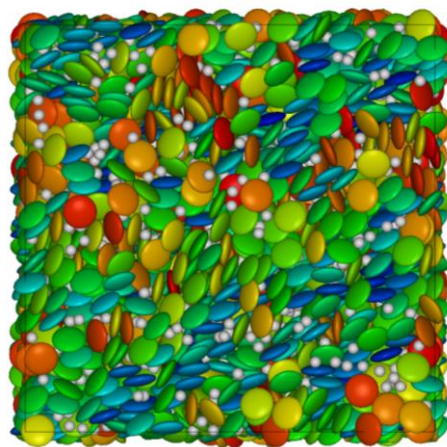
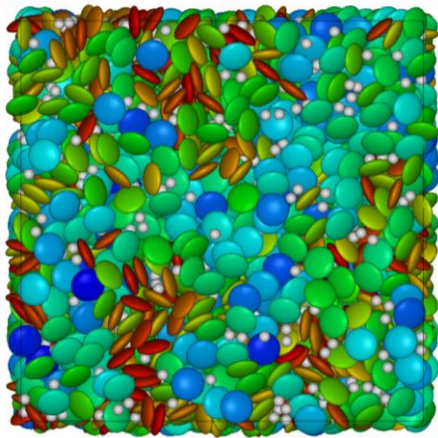
$T^*=2.75$



$T^*=6.00$



$T^*=9.25$



$T^*=10.00$

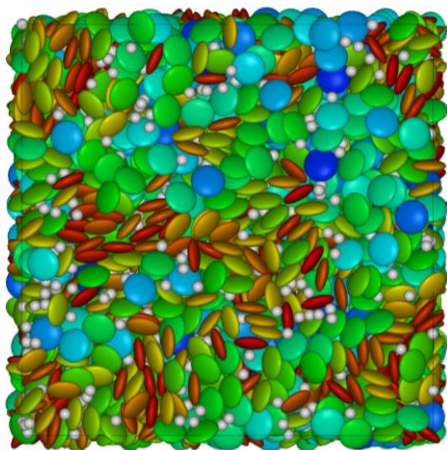


Figure S 25 Snapshots of the GB:LJ=2:1 system, $q_{GB}^*=0.5$ at some selected T^*

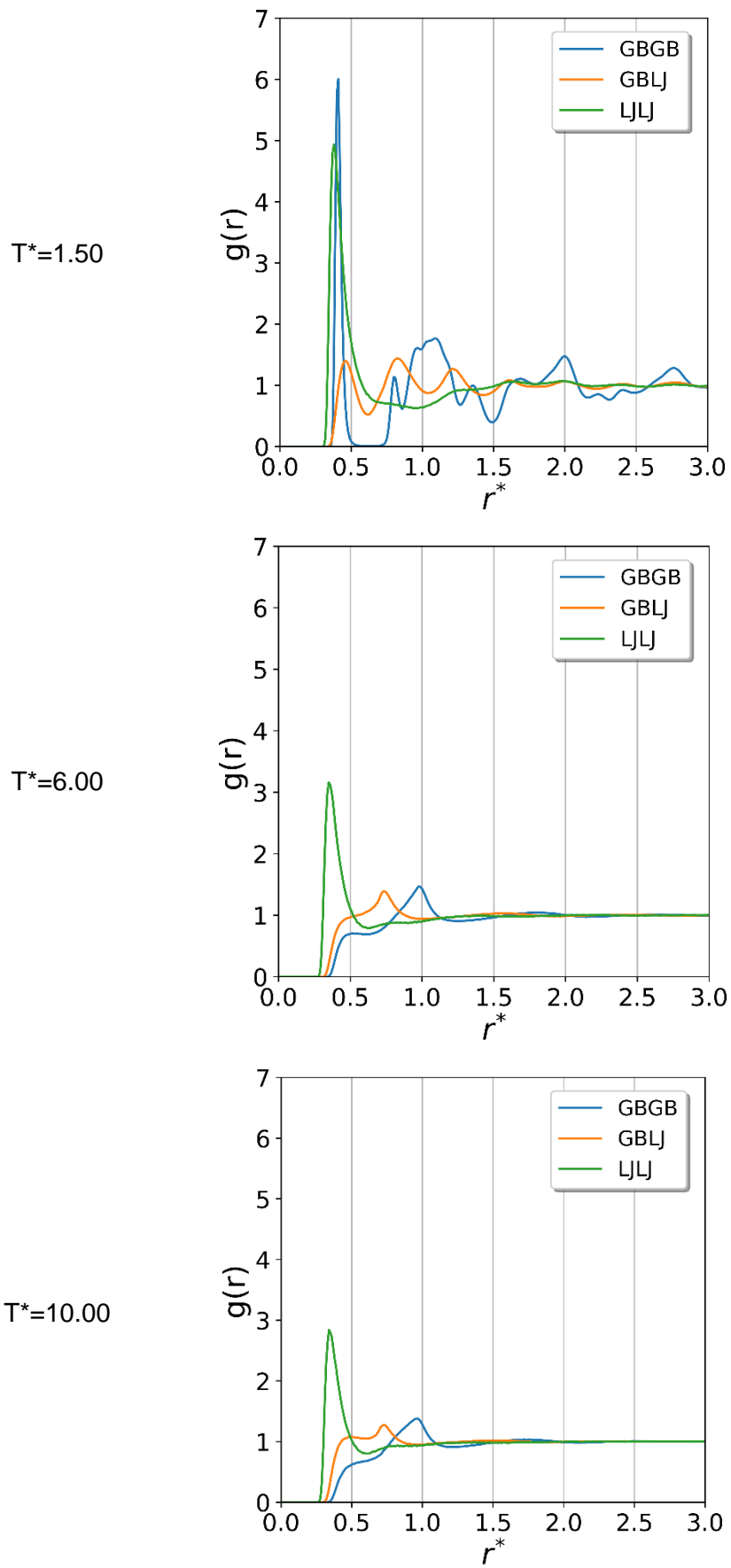


Figure S 26 Radial distribution functions, $g(r)$, of all the particle pairs for the columnar, nematic and isotropic phases, respectively on top, center and bottom

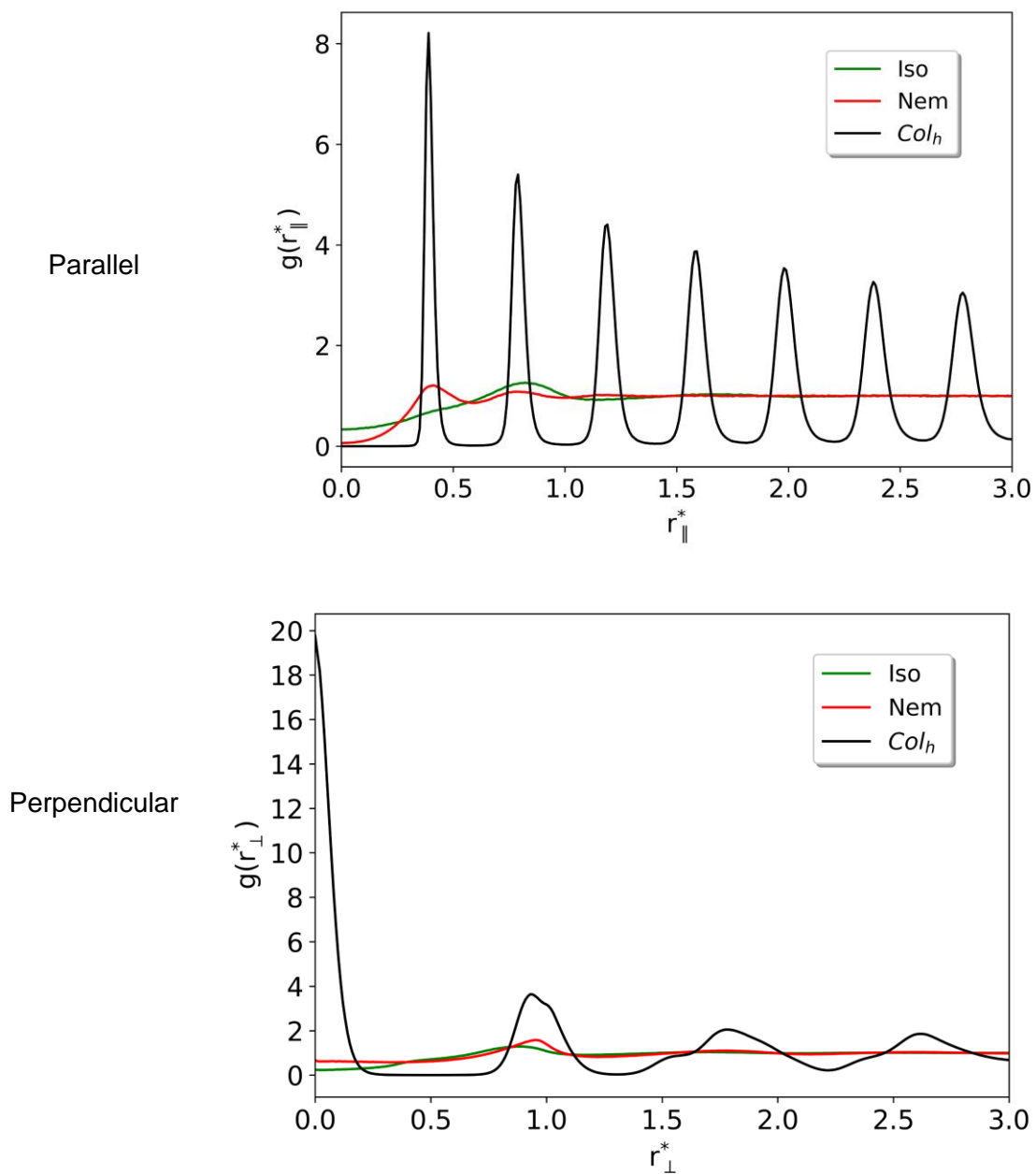


Figure S 27 Parallel, top, and perpendicular, bottom, radial distribution functions, $g(r_{\parallel}^*)$ and $g(r_{\perp}^*)$, of the discotic particles in the columnar (black), nematic (red) and isotropic phases (green). The temperatures of Iso, Nem and Col_h are 10.00, 6.00 and 1.50 respectively

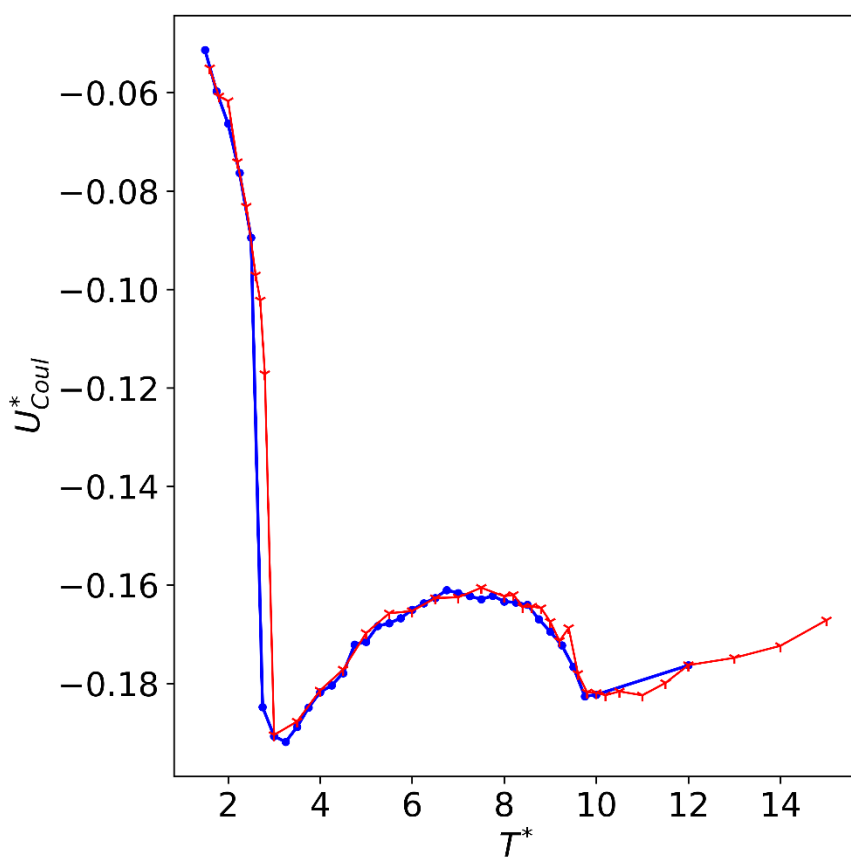
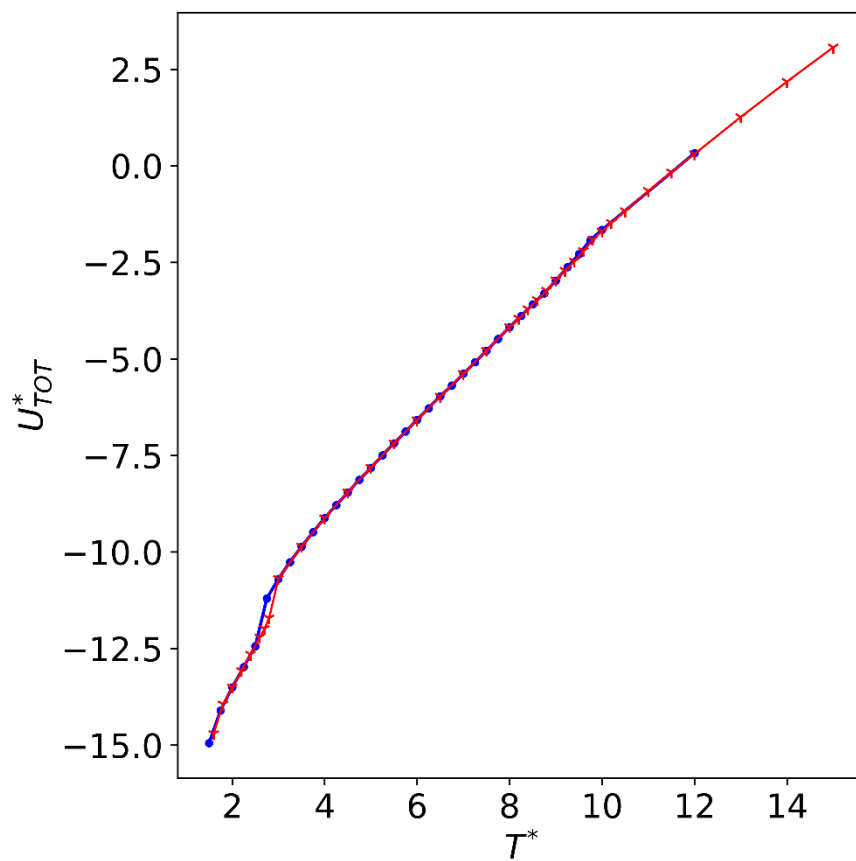
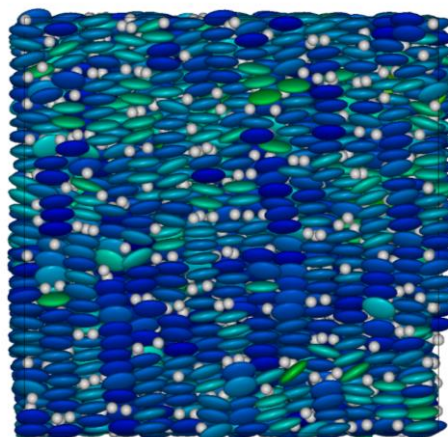
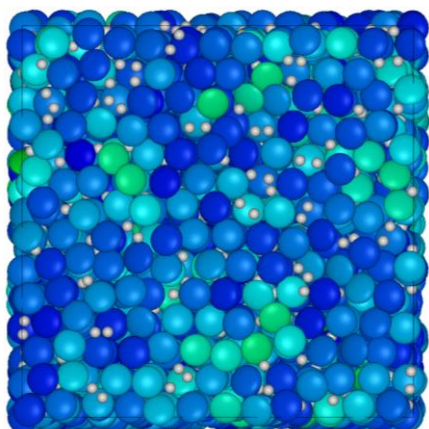


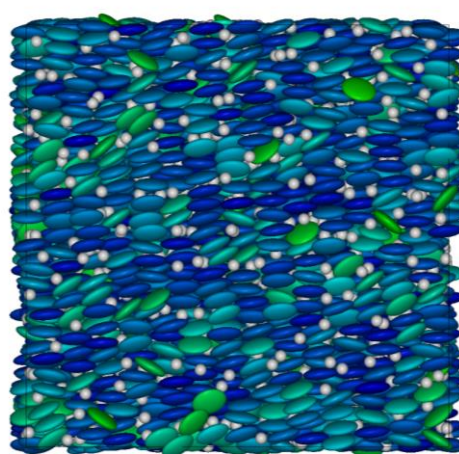
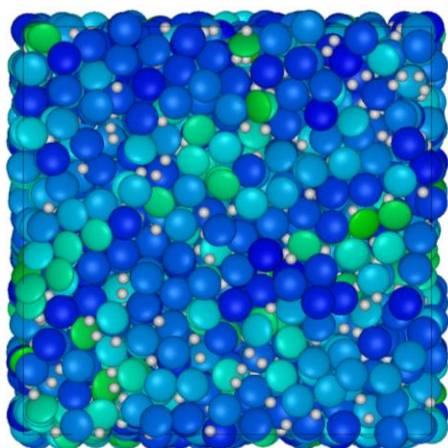
Figure S 28 Total energy (U_{TOT}^*) and electrostatic energy (U_{Coul}^*) as a function of temperature for the GB:LJ=2:1 and $q_{GB}^*=0.5$ system. Heating runs are represented in red, while cooling runs are represented in blue

$$q_{GB}^* = 1.00$$

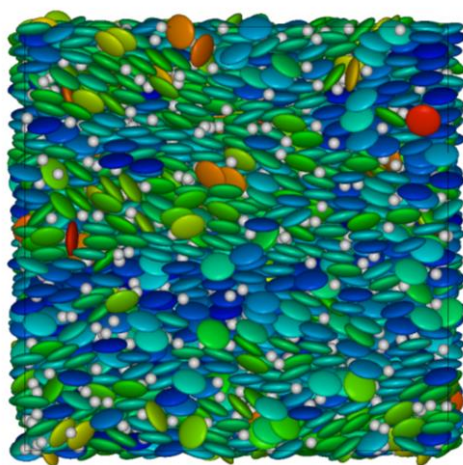
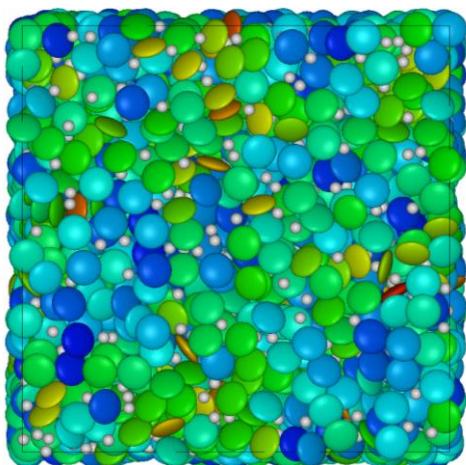
$T^*=1.25$



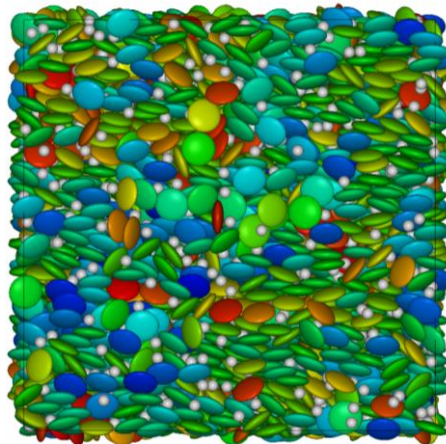
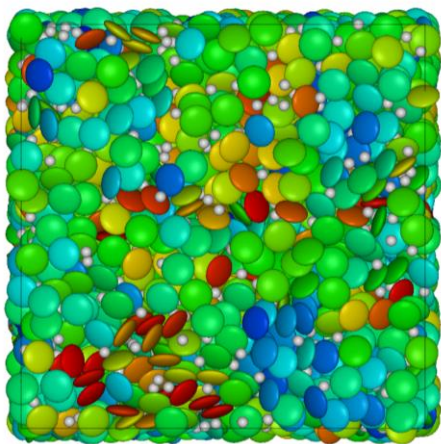
$T^*=2.00$



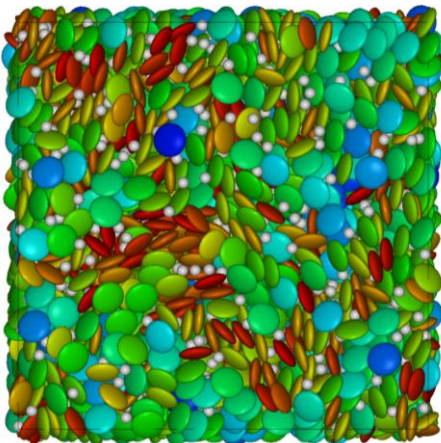
$T^*=4.00$



$T^*=6.50$



$T^*=8.00$



$T^*=10.00$

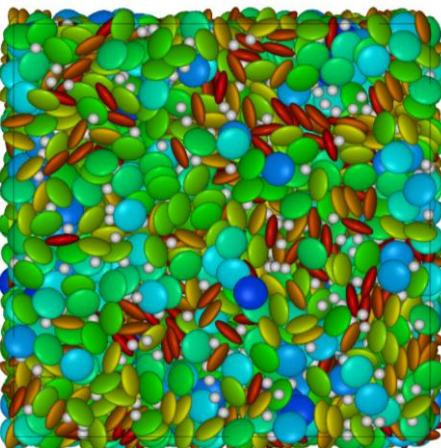


Figure S 29 Snapshots of the GB:LJ=2:1 system, $q_{GB}^*=1.0$ at some selected T^*

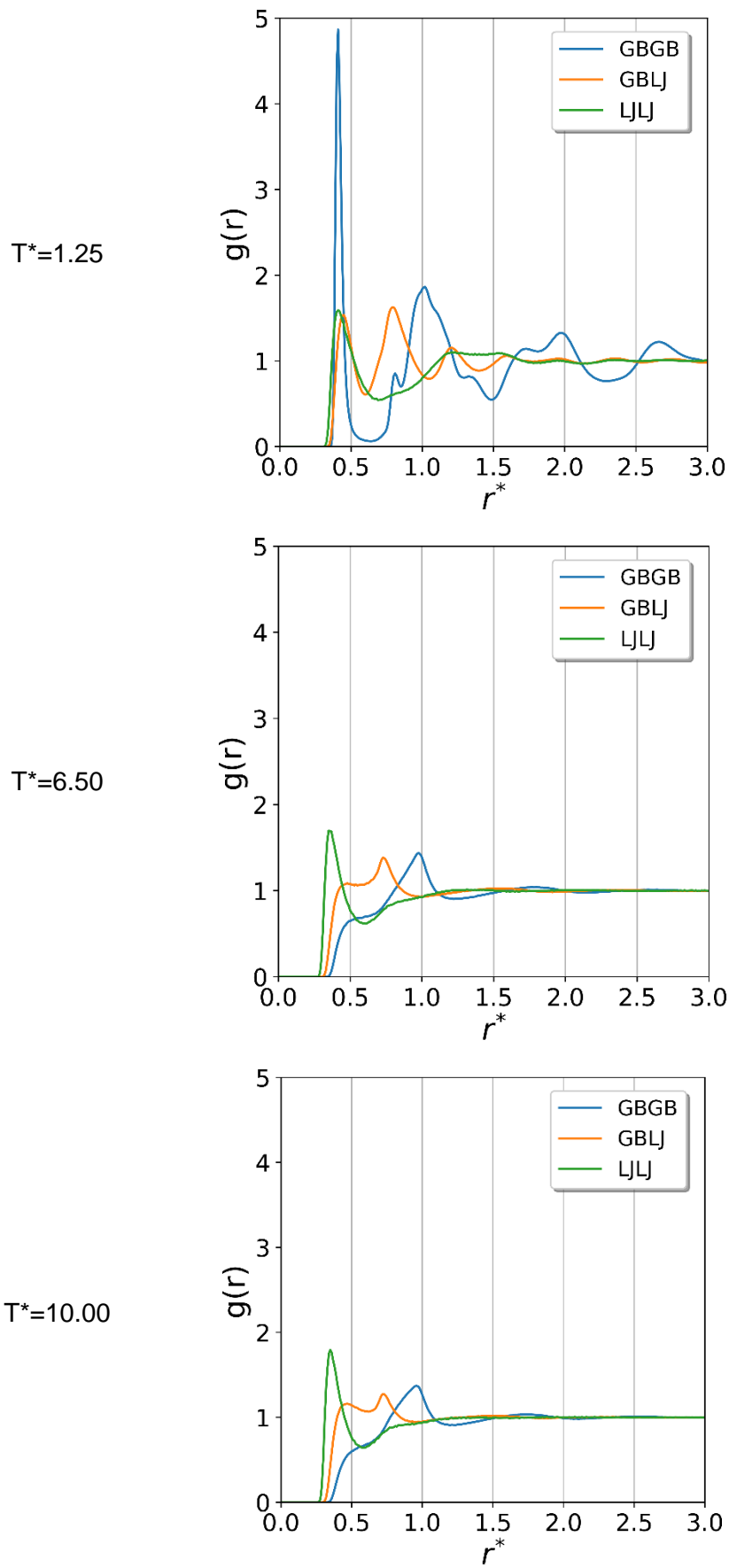


Figure S 30 Radial distribution functions, $g(r)$, of all the particle pairs for the columnar, nematic and isotropic phases, respectively on top, center and bottom.

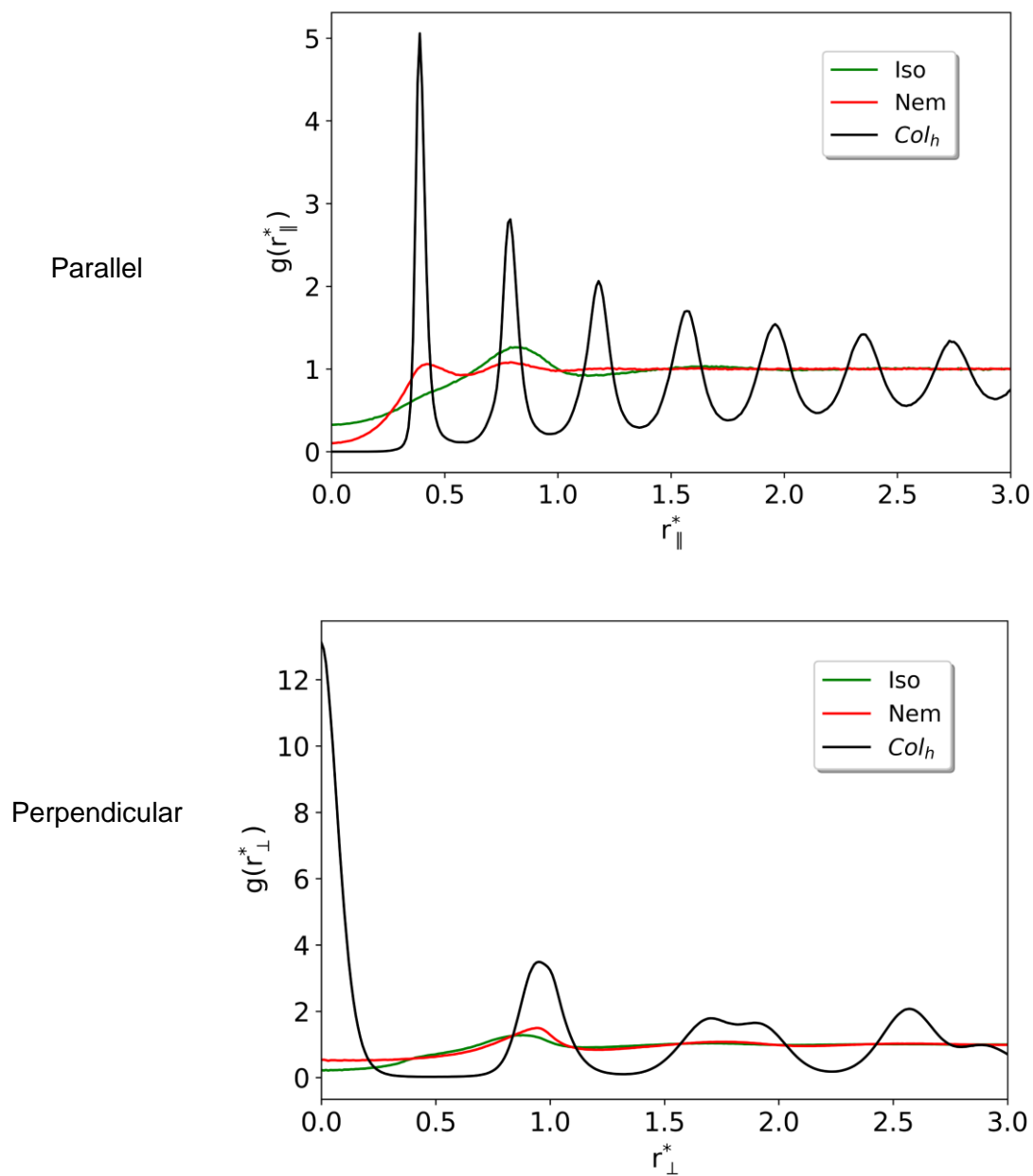


Figure S 31 Parallel, top, and perpendicular, bottom, radial distribution functions, $g(r_{\parallel}^*)$ and $g(r_{\perp}^*)$, of the discotic particles in the columnar (black), nematic (red) and isotropic phases (green). The temperatures of Iso, Nem and Col_h are 10.00, 6.50 and 1.25 respectively

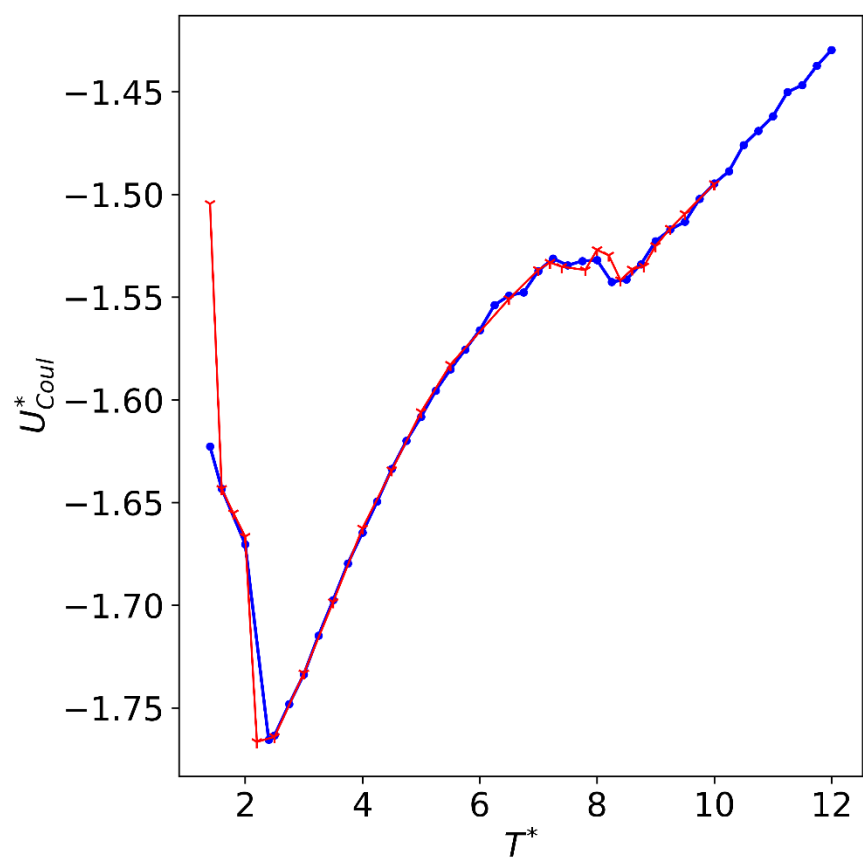
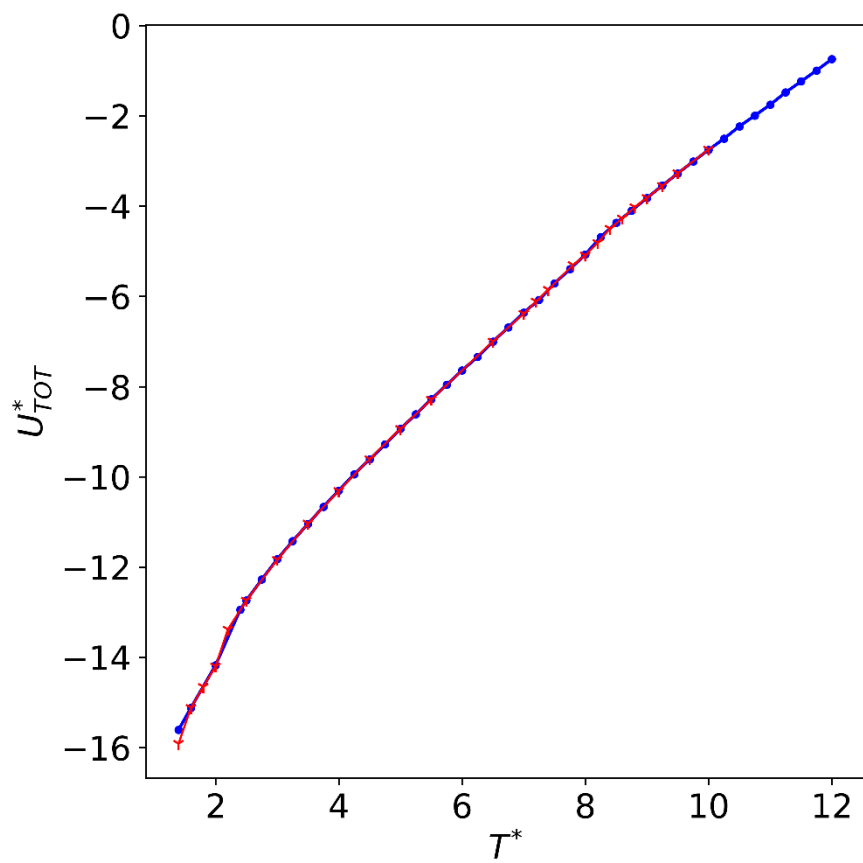
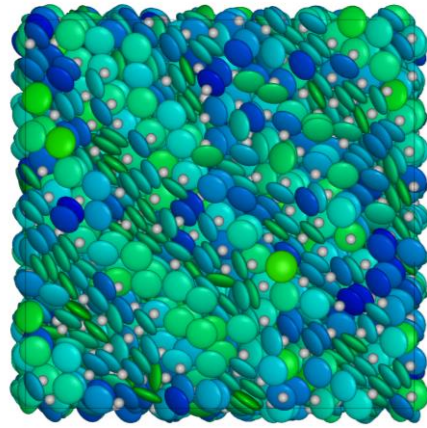
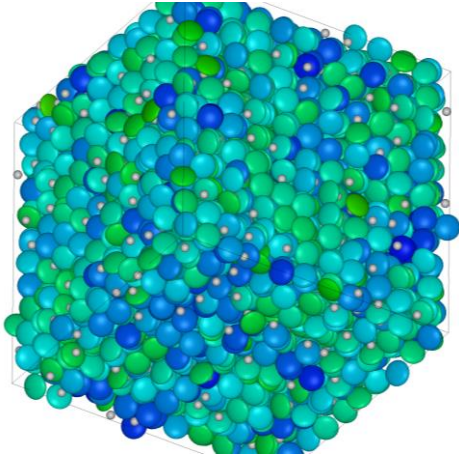


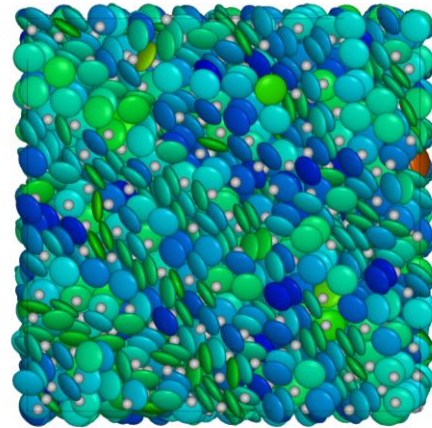
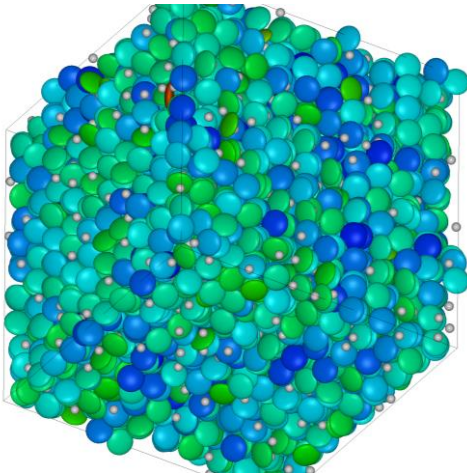
Figure S 32 Total energy (U_{TOT}^*) and electrostatic energy (U_{Coul}^*) as a function of temperature for the GB:LJ=2:1 and $q_{GB}^*=1.0$ system. Heating runs are represented in red, while cooling runs are represented in blue

$$q_{GB}^* = 2.00$$

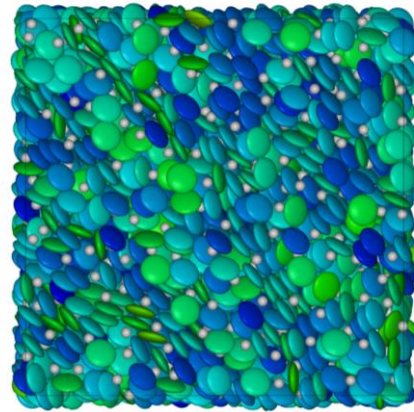
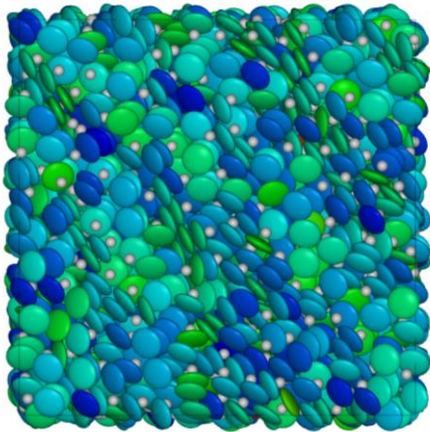
$T^*=1.20$



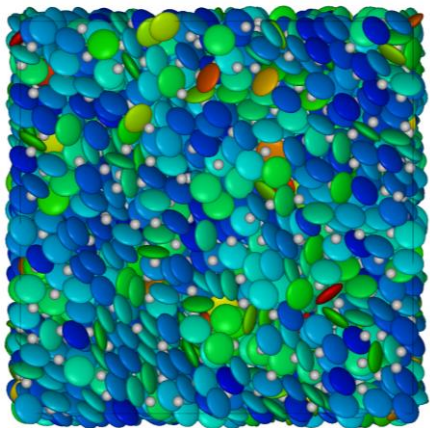
$T^*=1.60$



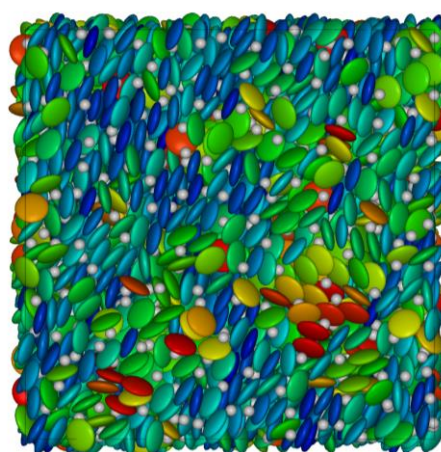
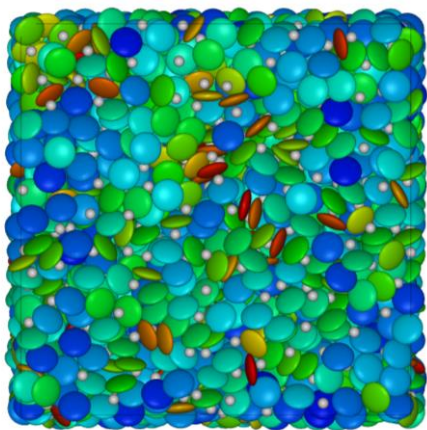
$T^*=1.80$



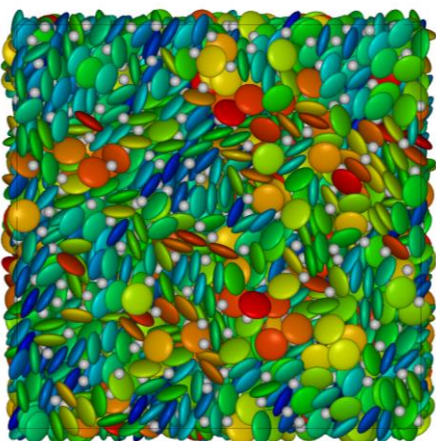
$T^*=2.00$



$T^*=3.00$



$T^*=4.00$



$T^*=5.40$

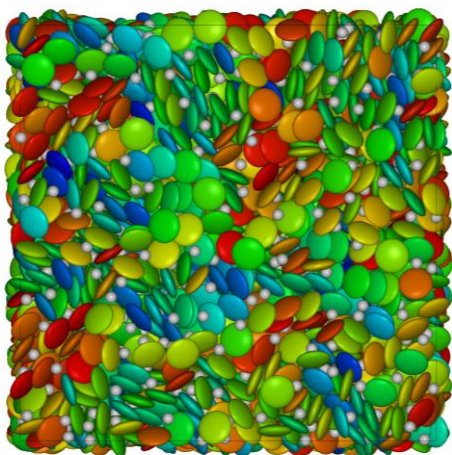


Figure S 33 Snapshots of the GB:LJ=2:1 system, $q_{GB}^*=2.0$ at some selected T^*

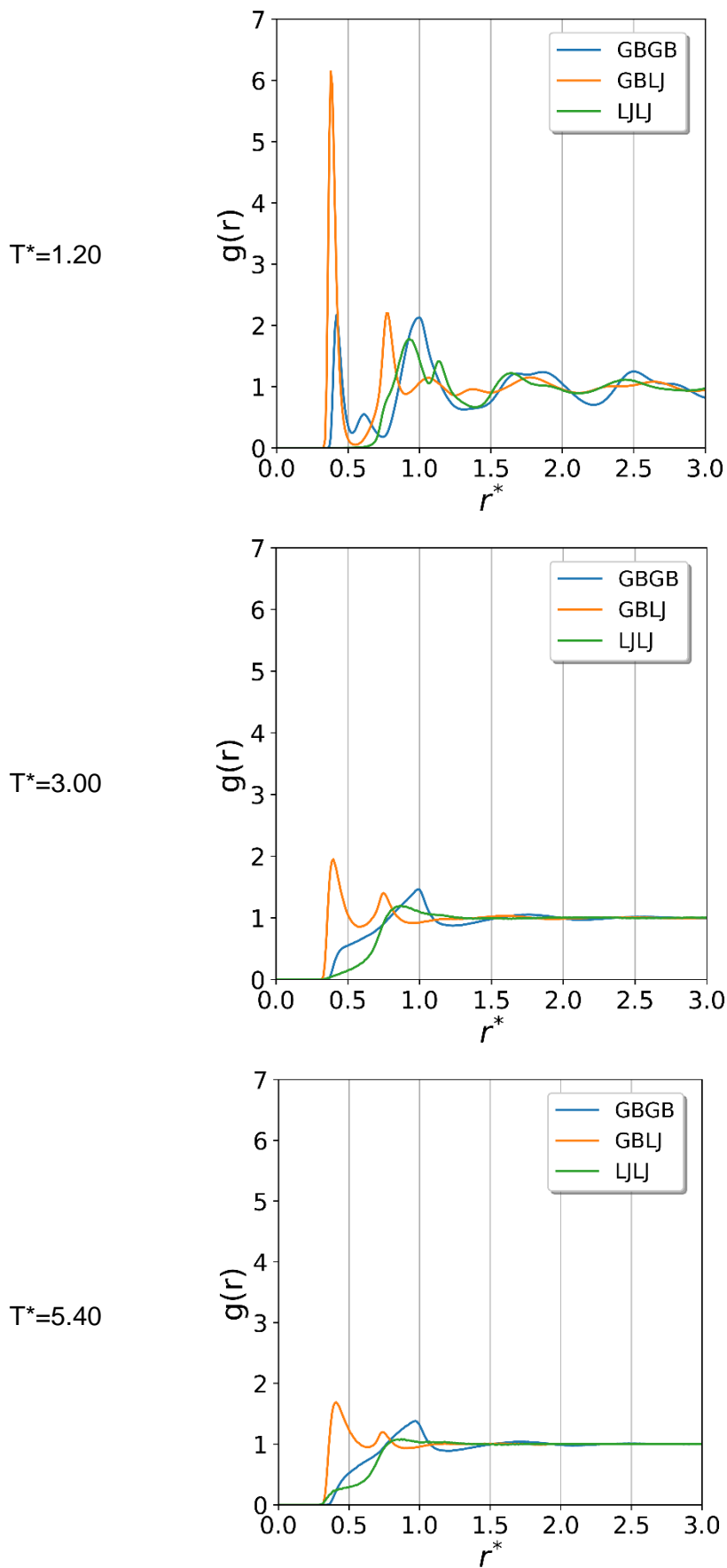


Figure S 34 Radial distribution functions, $g(r)$, of all the particle pairs for the columnar, nematic and isotropic phases, respectively on top, center and bottom

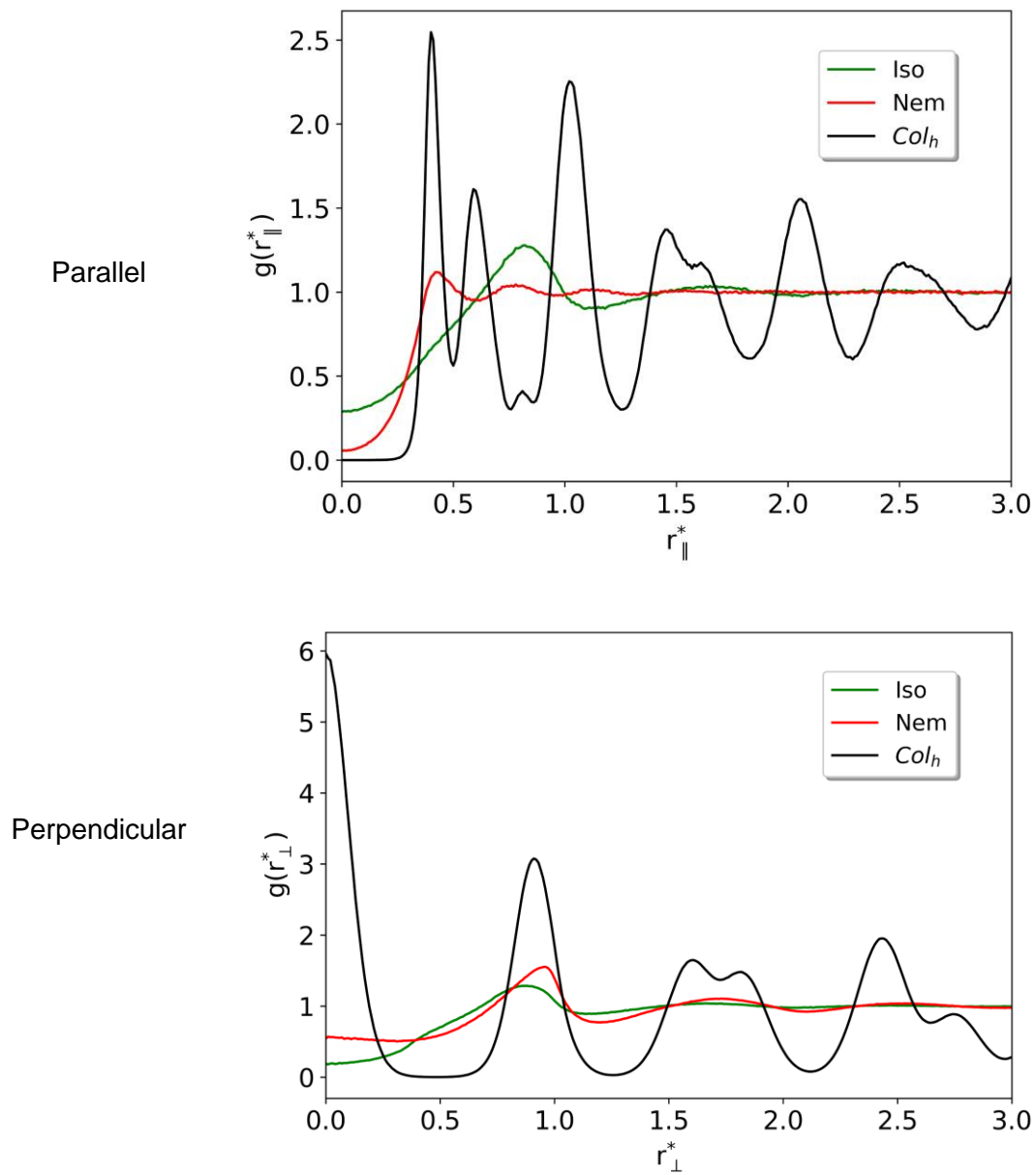


Figure S 35 Parallel, top, and perpendicular, bottom, radial distribution functions, $g(r_{\parallel}^*)$ and $g(r_{\perp}^*)$, of the discotic particles in the columnar (black), nematic (red) and isotropic phases (green). The temperatures of Iso, Nem and Col_h are 5.40, 3.00 and 1.20 respectively

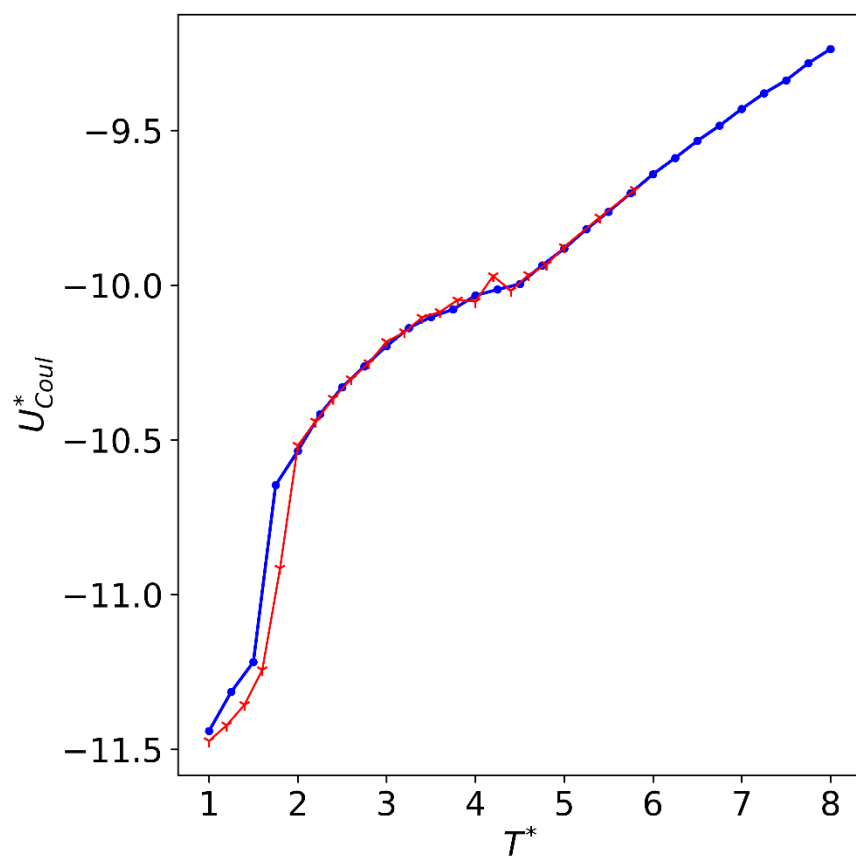
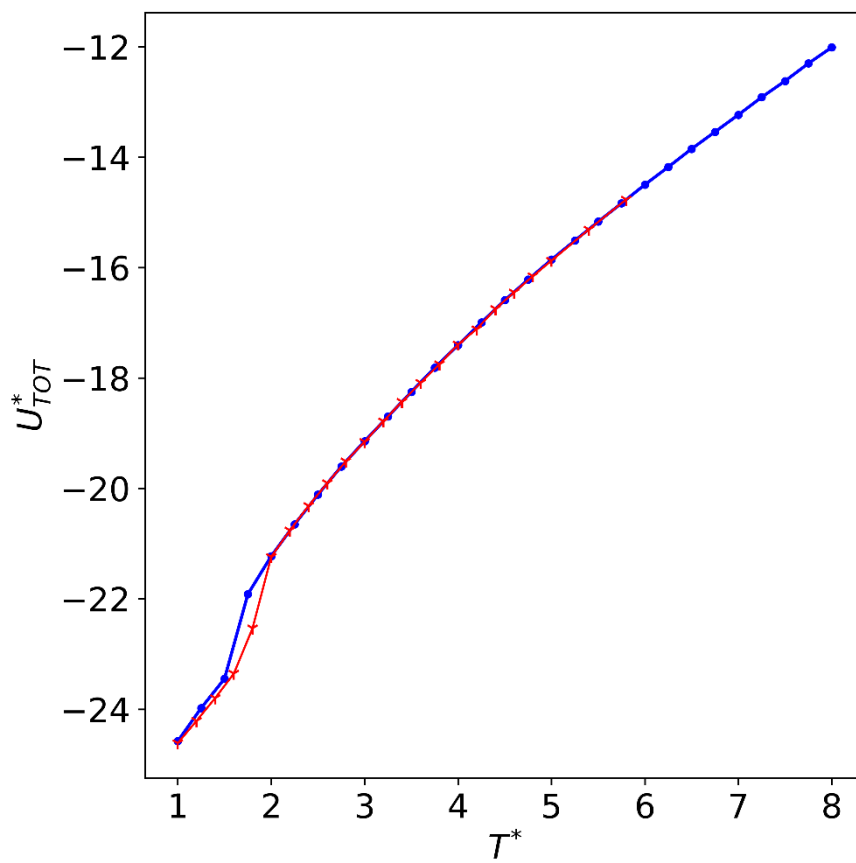


Figure S 36 Total energy (U_{TOT}^*) and electrostatic energy (U_{Coul}^*) as a function of temperature for the GB:LJ=2:1 and $q_{GB}^*=2.0$ system. Heating runs are represented in red, while cooling runs are represented in blue

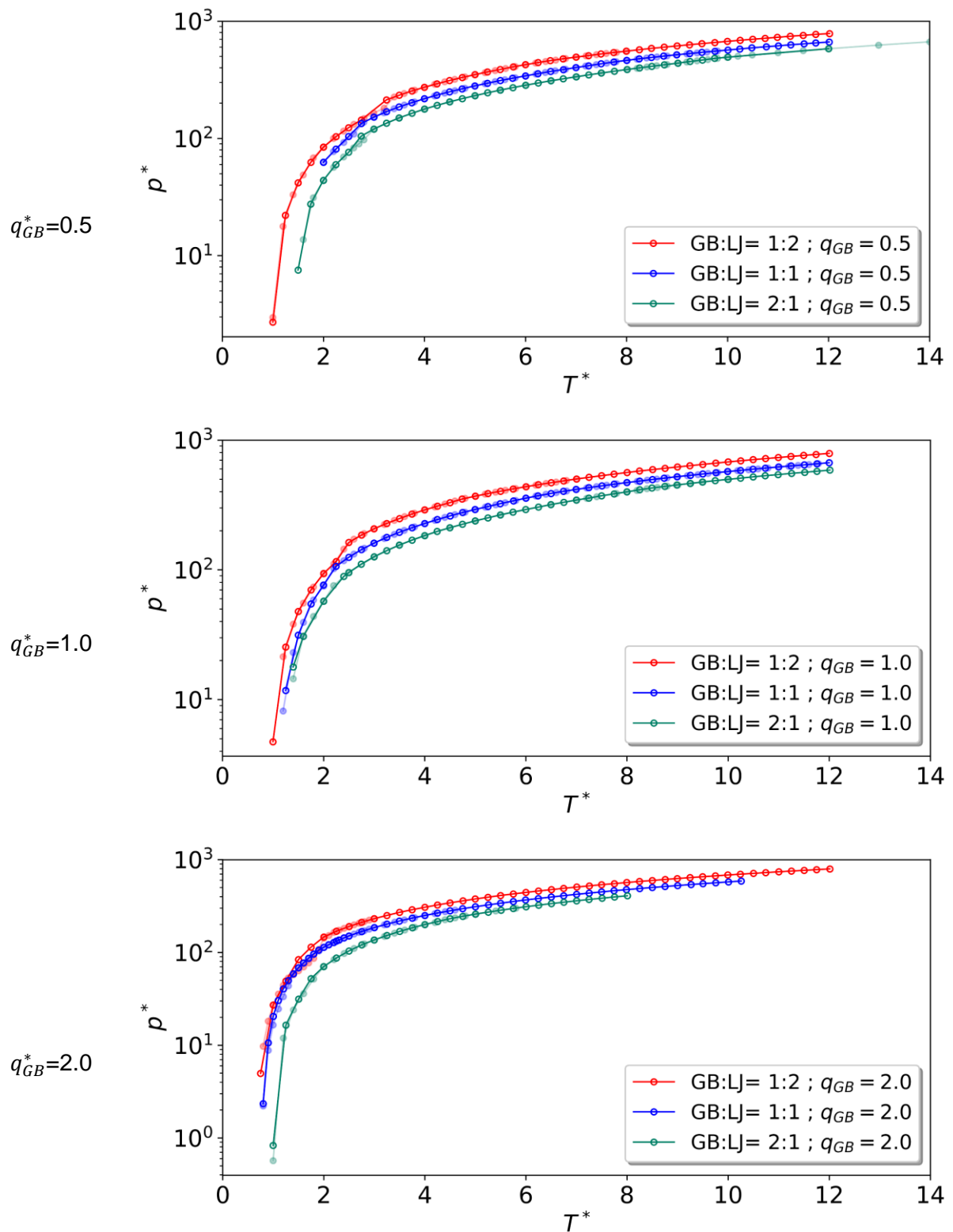


Figure S 37 Pressure-Temperature (p^*-T^*) diagram for all the studied systems grouped by charge. The pressure is represented using a logarithmic scale. On the top the $q_{GB}^*=0.5$ is reported, while in the center and bottom the two charges are $q_{GB}^*=1.0$ and $q_{GB}^*=2.0$ respectively. The red, blue and green colors are used to represent GB:LJ=1:2, GB:LJ=1:1 and GB:LJ=2:1 systems respectively. Heating and cooling runs, depicted with solid and transparent markers, perfectly overlap