Electronic Supplementary Information (ESI) for Temperature-driven self-assembly in a hexagonal mesophase-forming model: a dynamic and structural study.

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1 LAMMPS Input Scripts

This section includes the necessary LAMMPS input scripts used in the simulations. The scripts provided here are designed for use with the Lennard-Jones units.

```
##### LOOP DIFERENTES T ######
variable x index 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8
clear
shell mkdir TT_${x}
variable y loop 1 8
label conf
units lj
boundary p p p
pair_style sw
neighbor 0.4 bin
neigh_modify every 1 delay 1
read_data DATA_$y_$x
pair_coeff  * * AB.sw A B
group A type 1
group B type 2
#IMPRESION DE DATOS ######
shell cd TT_${x}
thermo 50000
```

```
######## RUN A T ####
reset_timestep 0
fix 1 all nvt temp $x $x 1
dump  888  all custom 10000 Hex_0_$y_${x}.dump  id type x y z xu yu zu
dump_modify 888 sort id
run 1
unfix 1
undump 888
variable s equal logfreq(2,5,10)
dump  88  all custom 1 Hex_$y_${x}.dump  id type x y z xu yu zu
dump_modify 88 sort id every v_s
fix 1 all npt temp $x $x 1.0 iso 1.0 1.0 10.0
run 600000
unfix 1
undump 88
shell cd ..
next y
clear
jump CORRIDA_COMPLETA.lmp conf
#################################################
next x
jump CORRIDA_COMPLETA.lmp
#################################################
```

The files named `DATA_$y_$x` represent independent configurations (where y corresponds to different independent configurations) that have been equilibrated at each temperature x. The file containing the parameters for the Stillinger-Weber potential used in this hexagonal system, named AB.sw, is as follows:

```
#     epsilon sigma a lambda gamma   cos(theta)     A      B     p   q  tol
A A A 1.0 1.0 1.80 0 0  -0.3333333333   7.049556277 0.6022245584  4.0  0.0  0.0
A A B 1.0 1.0 1.80 0 0  -0.3333333333   7.049556277 0.6022245584  4.0  0.0  0.0
A B A 1.0 1.0 1.80 0 0  -0.3333333333   7.049556277 0.6022245584  4.0  0.0  0.0
A B B 2.0 1.15 1.80 0 0  -0.3333333333   7.049556277 0.6022245584  4.0  0.0  0.0
B B B 1.0 1.0 1.80 0 0  -0.3333333333   7.049556277 0.6022245584  4.0  0.0  0.0
B B A 1.0 1.0 1.80 0 0  -0.3333333333   7.049556277 0.6022245584  4.0  0.0  0.0
B A B 1.0 1.0 1.80 0 0  -0.3333333333   7.049556277 0.6022245584  4.0  0.0  0.0
B A A 2.0 1.15 1.80 0 0  -0.3333333333   7.049556277 0.6022245584  4.0  0.0  0.0
```

2 LAMMPS Input Scripts

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Contact Information

For any questions regarding the data or scripts, please contact the authors at cbalbuena@fi.mdp.edu.ar.