**Code and curves of unsorted simulation:**

# ---------- Initialize Simulation ---------------------

units metal

atom\_style atomic

boundary p p p

newton on

dimension 3

# ---------- Create Atoms ---------------------

read\_data graphene10.data

# ---------- Define Interatomic Potential ---------------------

pair\_style airebo 3.0

pair\_coeff \* \* CH.airebo C

# ---------- Define Settings ---------------------

neighbor 2.0 nsq

neigh\_modify delay 1

timestep 0.0001 #measured in ps = 0.1 fs

thermo\_style custom step time atoms temp ke pe etotal vol press

thermo 1

compute 1 all pe/atom pair

# ---------- Relaxation ---------------------

min\_style fire

min\_modify dmax 0.01 line forcezero

minimize 1.0e-15 1.0e-15 1000000 10000000

# ---------- equilibration at 300 K ---------------------

velocity all create 300.0 4928459 dist gaussian units box

fix 1 all npt temp 300.0 300.0 0.01 iso 0.0 0.0 1

run 100000 #to have 10 ps equilibration

# write out restart of equilibration

write\_restart grapheneNPTeq.restart

unfix 1

#----------------------dumping files--------------------

shell mkdir dumpppf\_def

shell cd dumpppf\_def

dump xyzfile all xyz 1 dump-AIREBOppf.xyz

dump cfgfile all cfg 1 dump.AIREBOppf\_\*.cfg mass type xs ys zs x y z vx vy vz fx fy fz c\_1

dump\_modify cfgfile element C

# ---------- Dynamics ---------------------

fix 2 all nve

run 20000

write\_restart grapheneNVE.restart

unfix 2

undump xyzfile

undump cfgfile

shell cd ..





**Code and curves of Sorted simulation:**

# ---------- Initialize Simulation ---------------------

units metal

atom\_style atomic

boundary p p p

newton on

dimension 3

# ---------- Create Atoms ---------------------

read\_data graphene10.data

# ---------- Define Interatomic Potential ---------------------

pair\_style airebo 3.0

pair\_coeff \* \* CH.airebo C

# ---------- Define Settings ---------------------

neighbor 2.0 nsq

neigh\_modify delay 1

timestep 0.0001 #measured in ps = 0.1 fs

thermo\_style custom step time atoms temp ke pe etotal vol press

thermo 1

compute 1 all pe/atom pair

# ---------- Relaxation ---------------------

min\_style fire

min\_modify dmax 0.01 line forcezero

minimize 1.0e-15 1.0e-15 1000000 10000000

# ---------- equilibration at 300 K ---------------------

velocity all create 300.0 4928459 dist gaussian units box

fix 1 all npt temp 300.0 300.0 0.01 iso 0.0 0.0 1

run 100000 #to have 10 ps equilibration

# write out restart of equilibration

write\_restart grapheneNPTeq.restart

unfix 1

#----------------------dumping files--------------------

shell mkdir dumpppf\_def

shell cd dumpppf\_def

dump xyzfile all xyz 1 dump-AIREBOppf.xyz

dump\_modify xyzfile element C

dump cfgfile all cfg 1 dump.AIREBOppf\_\*.cfg mass type xs ys zs x y z vx vy vz fx fy fz c\_1

dump\_modify cfgfile sort id element C

# ---------- Dynamics ---------------------

fix 2 all nve

run 20000 #to have 2 ps production

write\_restart grapheneNVE.restart

unfix 2

undump xyzfile

undump cfgfile

shell cd ..



