# ReaxFF potential for TATB system

# this run is equivalent to reax/in.reax.tatb,

units real

boundary p p p

atom\_style charge

read\_restart coro-oh.restart.100000

pair\_style reax/c NULL

pair\_coeff \* \* ffield.reax C H O

compute reax all pair reax/c

variable eb equal c\_reax[1]

variable ea equal c\_reax[2]

variable elp equal c\_reax[3]

variable emol equal c\_reax[4]

variable ev equal c\_reax[5]

variable epen equal c\_reax[6]

variable ecoa equal c\_reax[7]

variable ehb equal c\_reax[8]

variable et equal c\_reax[9]

variable eco equal c\_reax[10]

variable ew equal c\_reax[11]

variable ep equal c\_reax[12]

variable efi equal c\_reax[13]

variable eqeq equal c\_reax[14]

neighbor 2.5 bin

neigh\_modify delay 0 every 10 check no

fix 1 all nvt temp 165.78002 1000 10

fix 2 all qeq/reax 1 0.0 10.0 1.0e-6 reax/c

fix 4 all reax/c/bonds 100 bonds.reaxc

thermo 10000

thermo\_style custom step temp epair etotal press &

v\_eb v\_ea v\_elp v\_emol v\_ev v\_epen v\_ecoa &

v\_ehb v\_et v\_eco v\_ew v\_ep v\_efi v\_eqeq

timestep 0.1

dump 1 all custom 5000 dump.reaxc.coro id type q x y z

#dump 2 all image 5 image.\*.jpg type type &

# axes yes 0.8 0.02 view 60 -30

#dump\_modify 2 pad 3

#dump 3 all movie 5 movie.mpg type type &

# axes yes 0.8 0.02 view 60 -30

#dump\_modify 3 pad 3

fix 3 all reax/c/species 1 1 100 species.tatb

restart 100000 coro-oh.restart

run 2500000