

Low-pressure Plasma Cleaning of the Chemical Coating Surface with Organic Contamination: A Study Combining Experimental and Molecular Dynamics

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The supplementary information includes the lammps runtime environment Settings, runtime condition Settings and runtime code designed in the paper.

```
dimension          3
units              real                                # Energy: eV Distance: Angstrom
Mass: Kg Times: picosecond
boundary          p p f                                # p = periodic, f= fixed
atom_style        charge                               # Classical particles

read_data 120DBP.data

variable num_tep equal 250.0
variable num_vol equal 0.10
variable num_mol equal 100

region bot block INF INF INF INF -30 -25 units box
group bot_f region bot

group oil type 1 2 3 4 5 6 7
pair_style reaxff NULL #lmp_control
#pair_style reaxff lmp_control
pair_coeff * * ffield.reax.cho C C O O C C H O
#fix QEQ all qeq/reaxff 1 0.0 20.0 1.0e-1 reaxff

change_box all z delta 0 50 units box
#change_box all z delta -10 50 units box
#change_box all x delta -10 10 units box
#change_box all y delta -10 10 units box

region top block -5 5 -5 5 55 65 units box
group top type 8
```

```

#pair_style      reaxff  NULL #!!!!!!mp_control
#pair_coeff      * * ffield.reax.CHO  C C O O C C H O
#fix             QEQ all qeq/reaxff 1 0.0 20.0 1.0e-2 reaxff

neighbor         2 bin
#neigh_modify    delay 0 every 10 check yes
neigh_modify     every 10 delay 0 check no
timestep        0.25

fix  Set bot_f setforce 0.0 0.0 0.0

#!!!!!!setting
#comm_style      tiled
#balance         0.9 rcb
thermo          100

#dump            1 all atom 100 mini.xyz
#minimize        1e-8 1e-8 10000 10000
#undump          1

thermo_modify    lost ignore flush yes
fix             1 all nvt temp ${num_tep} ${num_tep} 10.0
fix             5 all qeq/reaxff 1 0.0 10.0 1e-6 reaxff #可以跑
#fix            5 all qeq/reaxff 1 0.0 20.0 1e-6 reaxff
fix             2 all temp/berendsen ${num_tep} ${num_tep} 100.0
fix             3 top nve

fix             4 top deposit 1000 8 ${num_mol} 12345 region top vz -
${num_vol} ${num_vol}
fix             zwalls all wall/reflect zlo EDGE

dump            dumpfil all custom 200 ${num_tep}-V${num_vol}-M${num_mol}.data
id type x y z
#dump           3 all custom 500 dump.atom.* id type q x y z

run            500000

```