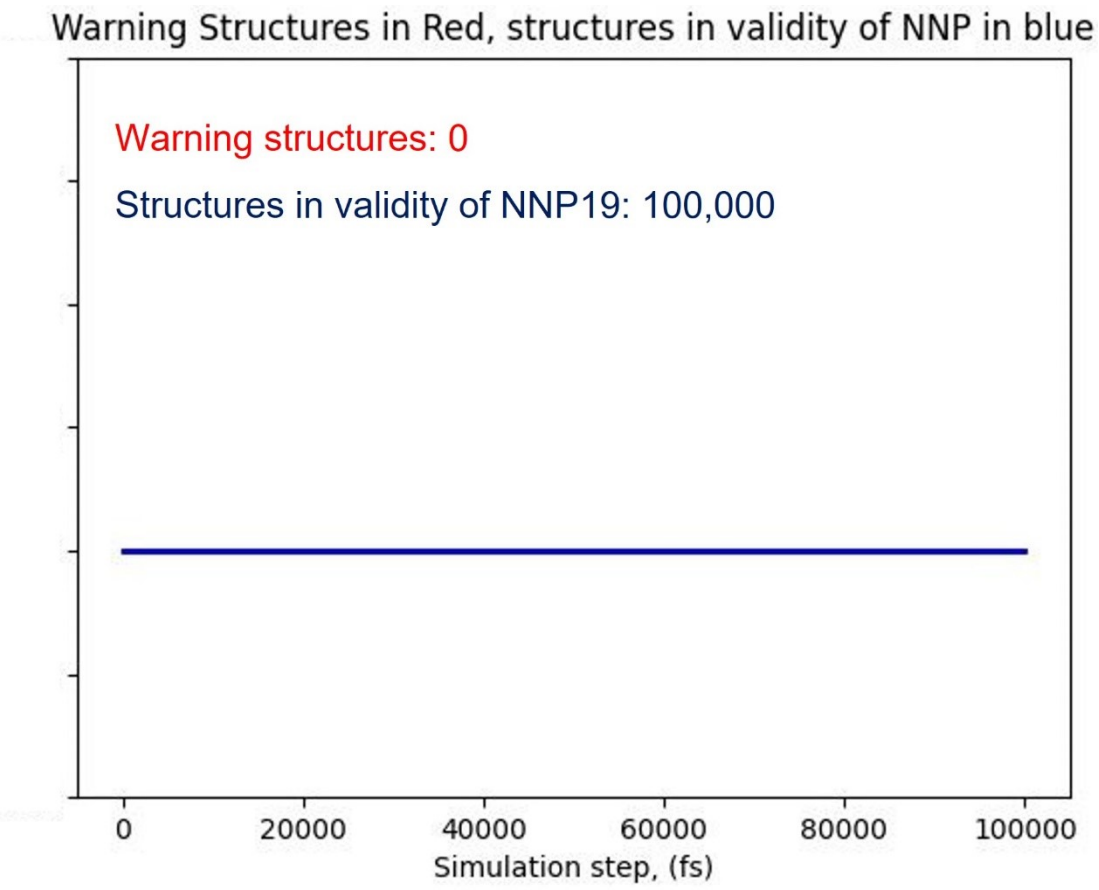

Simulation time: 100,000 fs

Total number of structures: 100,000

Warning structures: 0

Structures in validity of NNP19: 100,000

Molecular Dynamics input file

```
# general variables
variable        oxygen atom "type==1"
variable        Mn atom "type==2"
variable        Pt atom "type==3"
variable        temperature equal 500
variable        dt equal 0.001
# general settings
units           metal
atom_style      atomic
# read initial structure
read_data system.data
group O type 1
group Mn type 2
group Pt type 3
# set up timestep
reset_timestep  0
timestep        ${dt}
pair_style      nnp showew yes showewsum 0 maxew 100000 resetew yes dir
/home/energy/tharoo/project/Training_data/19nnp/100_ep cflength 1 cfenergy 1 emap "1:O,2:Mn,3:Pt"
pair_coeff      * * 6.01
#pair_coeff 3* 1*2 1.0 1.0 2.5
#Define bottom slab
region fixed_slab block EDGE EDGE EDGE EDGE EDGE 12.10
group slab region fixed_slab
# initialize velocitiesn
velocity        all create ${temperature} 12345 dist gaussian
#velocity to fix 3 bottom layers
velocity        slab set 0.0 0.0 0.0
fix 1 all plumed plumedfile plumed.dat outfile p.log
fix 2 all nvt temp 500.0 500 $(100.0*dt)
fix 3 slab setforce 0.0 0.0 0.0
```

```
dump            1 all custom 500 dump.lammps id type x y z vx vy vz fx fy fz
dump_modify     1 sort id
thermo_style    custom step pe ke temp etotal
thermo          1
run             100000
```

Plumed input file

CV used (local-CVs): Coordination number of an individual Mn atom and 4O

UNITS LENGTH=A ENERGY=eV TIME=fs

man: GROUP ATOMS=50

oxy: GROUP ATOMS=55,56,57,58

cn: COORDINATION GROUPA=oxy GROUPB=man R_0=1.8

metad: METAD ARG=cn SIGMA=0.05 HEIGHT=0.1 PACE=500 TEMP=500 BIASFACTOR=5

PRINT ARG=cn STRIDE=1 FILE=COLVAR

Coordinates of 2 Mn surface structure (Coordinates file for running MD)

58 atoms

3 atom types

0.00000000e+00 8.06346154e+00 xlo xhi

0.00000000e+00 6.98061123e+00 ylo yhi

0.00000000e+00 2.71866218e+01 zlo zhi

-4.03173076987692 0 0.20631670725752604 xy xz yz

Masses

1 15.999

2 54.938044

3 195.084

Atoms

1 3 9.30000000e-07 1.70447334e+00 7.16626169e+00

2 3 2.68781862e+00 1.70447210e+00 7.16626165e+00

3 3 5.37564153e+00 1.70446232e+00 7.16626674e+00

4 2 -1.34391372e+00 3.87182863e+00 7.16835863e+00

5 2 1.34390687e+00 3.87183380e+00 7.16836431e+00

6 2 4.03173857e+00 3.87182846e+00 7.16835934e+00

7 3 -2.68782002e+00 6.15755038e+00 7.31806821e+00

8 3 -8.00000000e-08 6.15754786e+00 7.31806919e+00

9 3 2.68781990e+00 6.15754785e+00 7.31806978e+00

10 3 1.34391053e+00 8.21223475e-01 9.52206995e+00

11 3 4.03172955e+00 8.21223125e-01 9.52207024e+00

12 3 6.71955188e+00 8.21224085e-01 9.52207011e+00

13 3 2.70000000e-07 3.19901000e+00 9.42905804e+00

14 3 2.68781898e+00 3.19900995e+00 9.42905694e+00

15 3 5.37564097e+00 3.19900959e+00 9.42905825e+00

16 3 -1.34390974e+00 5.48511236e+00 9.64631917e+00

17 3 1.34390894e+00 5.48511370e+00 9.64632016e+00

18 3 4.03173095e+00 5.48511559e+00 9.64631967e+00

19 2 -3.37000000e-06 -4.44970254e-02 1.18050827e+01

20 2 2.68782230e+00 -4.44926154e-02 1.18050851e+01

21 2 5.37564524e+00 -4.44931254e-02 1.18050843e+01

22 3 -1.34391142e+00 2.31934642e+00 1.17370896e+01

23 3 1.34390958e+00 2.31934546e+00 1.17370916e+01

24 3 4.03173030e+00 2.31934684e+00 1.17370922e+01

25 2 -2.68782420e+00 4.96615787e+00 1.17381062e+01

26 2 1.81000000e-06 4.96616054e+00 1.17381083e+01

27 2 2.68782168e+00 4.96615698e+00 1.17381063e+01

28 3 2.76153700e-02 1.60850322e+00 1.39263670e+01

29 3 9.85311000e-03 1.74777246e-02 1.82711077e+01

30 3 1.40561055e+00 7.53988995e-01 1.59032578e+01

31 2 2.72501988e+00 1.39194611e+00 1.38675546e+01

32 3 2.71864824e+00 6.43993646e-02 1.81395719e+01

33 2 3.91812346e+00 6.75201185e-01 1.58684449e+01

34 3 5.29233211e+00 1.48647738e+00 1.39261548e+01

35 3 5.37342900e+00 -3.37243554e-02 1.82001550e+01

36 2 6.74449204e+00 9.19262365e-01 1.60415989e+01

37 3 -1.31662814e+00 4.15129802e+00 1.38186714e+01

38 3 -1.28708287e+00 2.36389447e+00 1.81768683e+01

39 2 -6.65634600e-02 3.26894319e+00 1.61418699e+01

40 3 1.33077536e+00 3.99806739e+00 1.37875862e+01

41 3 1.34517441e+00 2.53110974e+00 1.82711626e+01

42 3 2.66770202e+00 3.10803421e+00 1.60140180e+01

43 3 4.04737607e+00 4.00443898e+00 1.37708786e+01

44 3 4.02516315e+00 2.41845209e+00 1.82119012e+01

45 3 5.45800767e+00 3.15616794e+00 1.59550845e+01

46 2 -2.56812807e+00 6.38569666e+00 1.37048547e+01

47 3 -2.59916253e+00 4.72778391e+00 1.82254538e+01

48 2 -1.17218807e+00 5.54654265e+00 1.60415696e+01

49 2 -1.65686710e-01 6.37226659e+00 1.38055382e+01

50 2 4.96778000e-02 4.67585009e+00 1.81206624e+01

51 3 1.29642268e+00 5.52275875e+00 1.60366352e+01

52 3 2.73018612e+00 6.29889951e+00 1.38686500e+01

53 2 2.61933008e+00 4.73040519e+00 1.85109844e+01

54 3 3.99879774e+00 5.48670796e+00 1.61177506e+01

55 1 -8.38284260e-01 4.64901185e+00 1.95485382e+01

56 1 2.76844688e+00 4.72967129e+00 2.00611836e+01

57 1 5.33386643e+00 1.52501095e+00 1.95515601e+01

58 1 1.29184779e+00 9.60912345e-01 1.96010900e+01