

1 CONTROL

DLPOLY: LiNbO3

```
temperature 2000.000000
pressure 0.000000
steps 100000
equilibration 30000
print every 500
stats every 500
timestep 0.0004000000 ps
ensemble nst ber 0.500000 0.500000 (ps)
traj 1 500 0
rdf 1000
multiple step 1
cap 1000
scale 307
primary cutoff 10.000
cutoff 10.000
delr width 1.000
rvdw cutoff 10.000
ewald precision 1.0E-6
shake tolerance 1.0E-6
quaternion tolerance 1.0E-5
job time 1520000
close time 200
finish
```

2 result

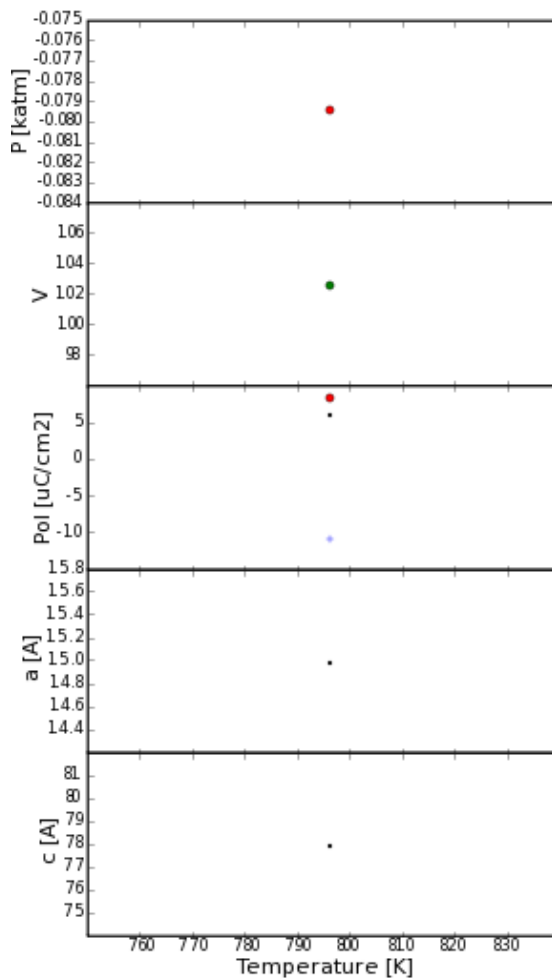


Figure 1: Pressure, Volume, Polarization verse temperature for MD simulation of LiNbO3 (test -c).

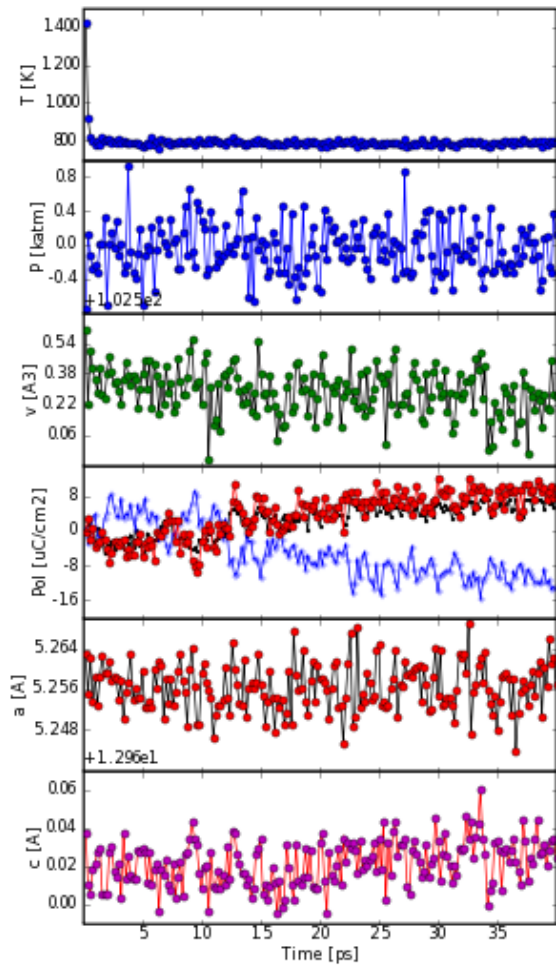


Figure 2: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO₃ at target temperature T=800 K (test).