

# 1 CONTROL

DLPOLY: LiNbO3

```
temperature 1200.000000
pressure 0.000000
steps 200000
equilibration 0
print every 500
stats every 500
timestep 0.0002000000 ps
ensemble nst hoover 0.040000 0.020000 (ps)
traj 1 500 0
multiple step 1
cap 1000
scale 200
primary cutoff 10.000
cutoff 10.000
delr width 0.5
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

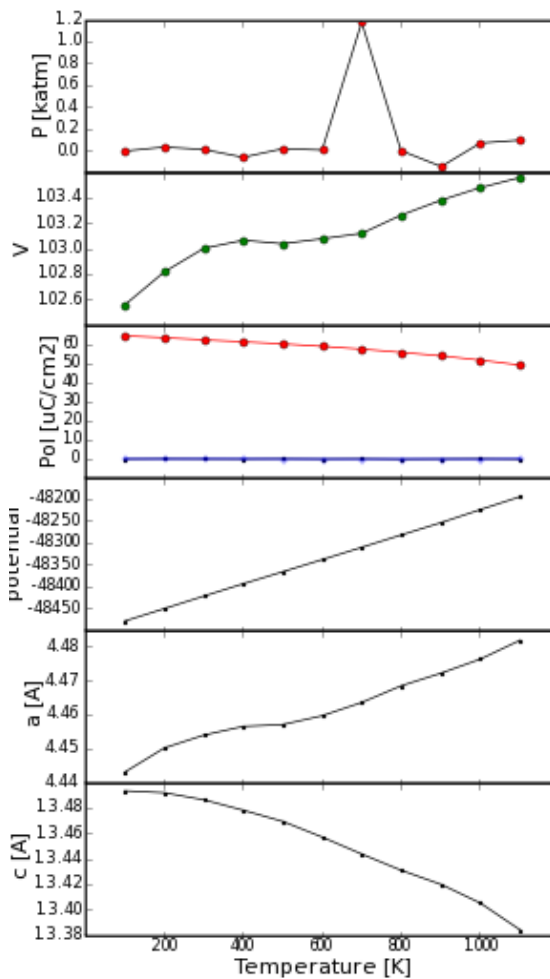


Figure 1: Pressure, Volume, Polarization verse temperature for MD simulation of LiNbO3 (new20081030 -d).

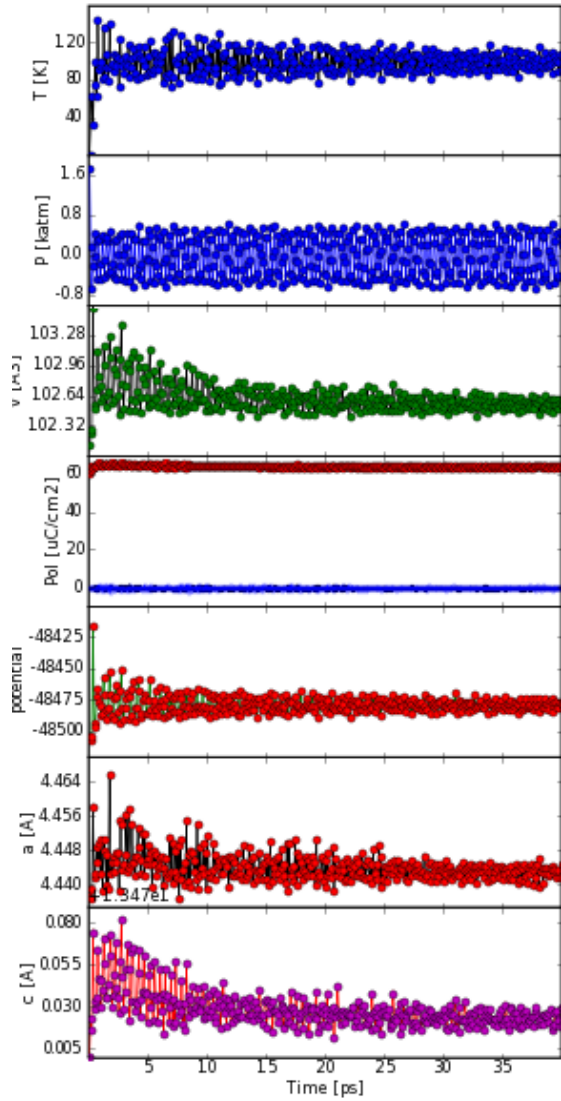


Figure 2: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=100$  K (new20081030).

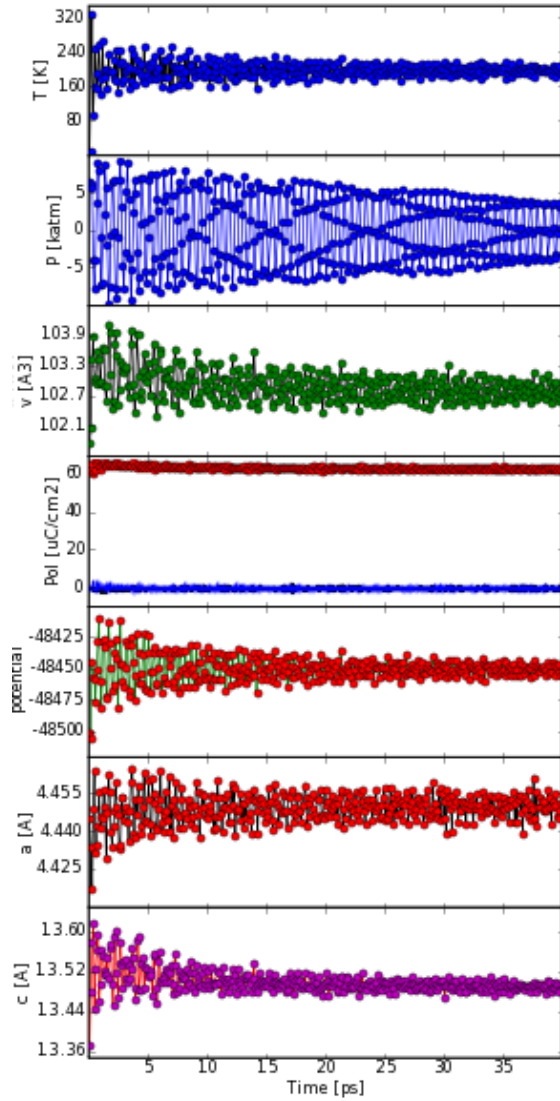


Figure 3: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=200$  K (new20081030).

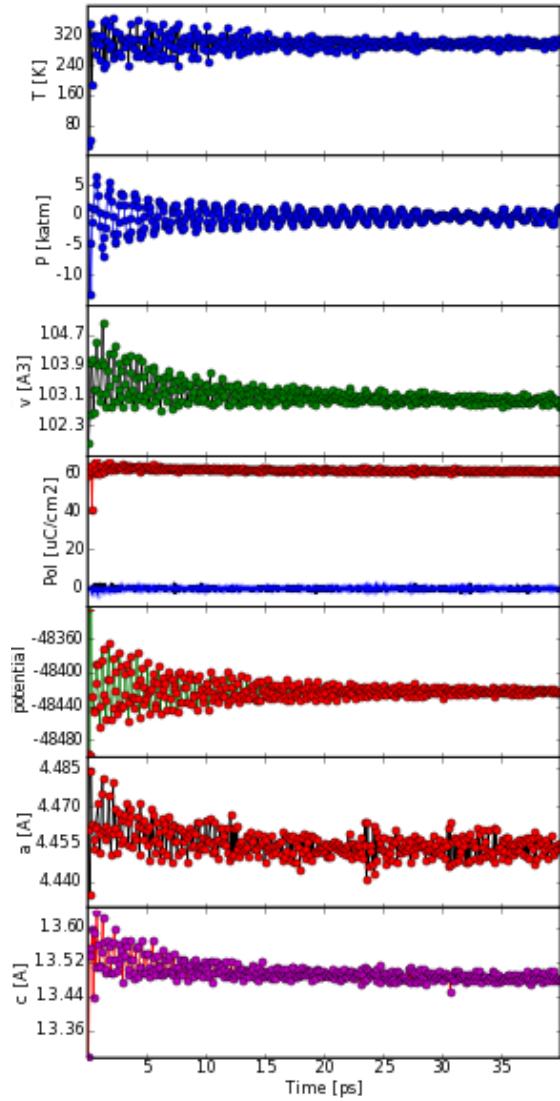


Figure 4: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=300$  K (new20081030).

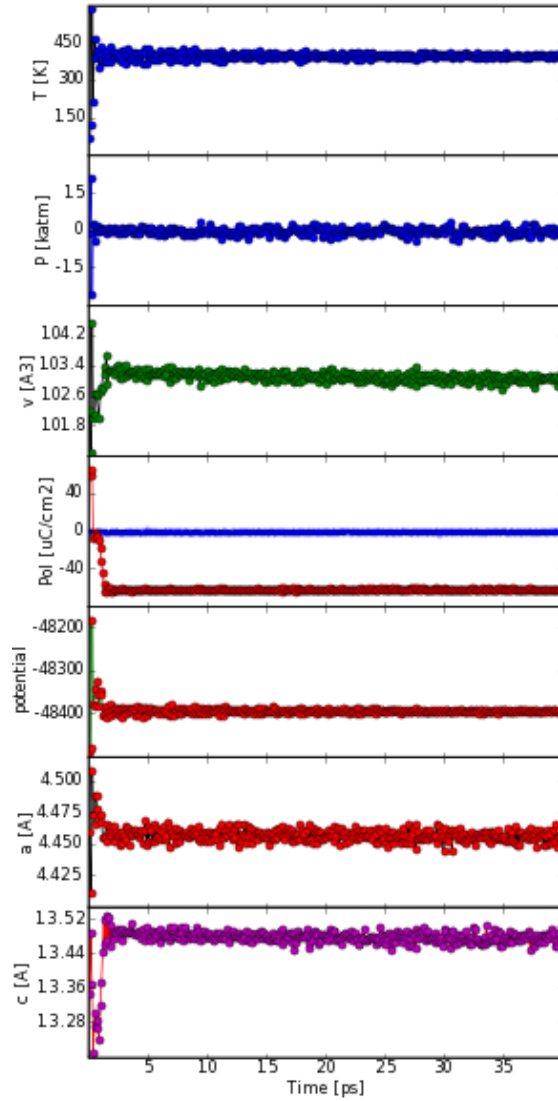


Figure 5: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=400$  K (new20081030).

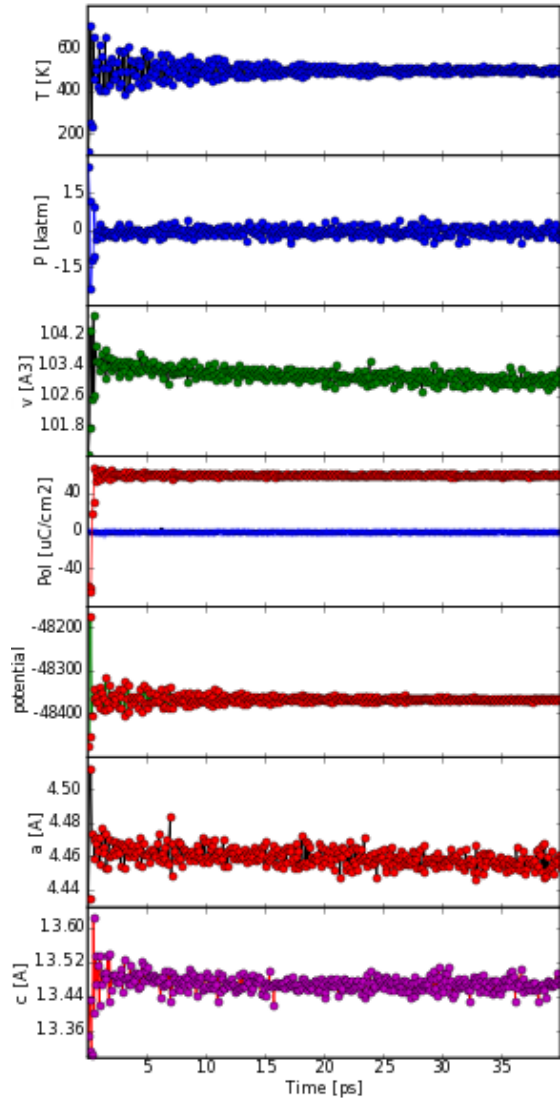


Figure 6: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=500$  K (new20081030).

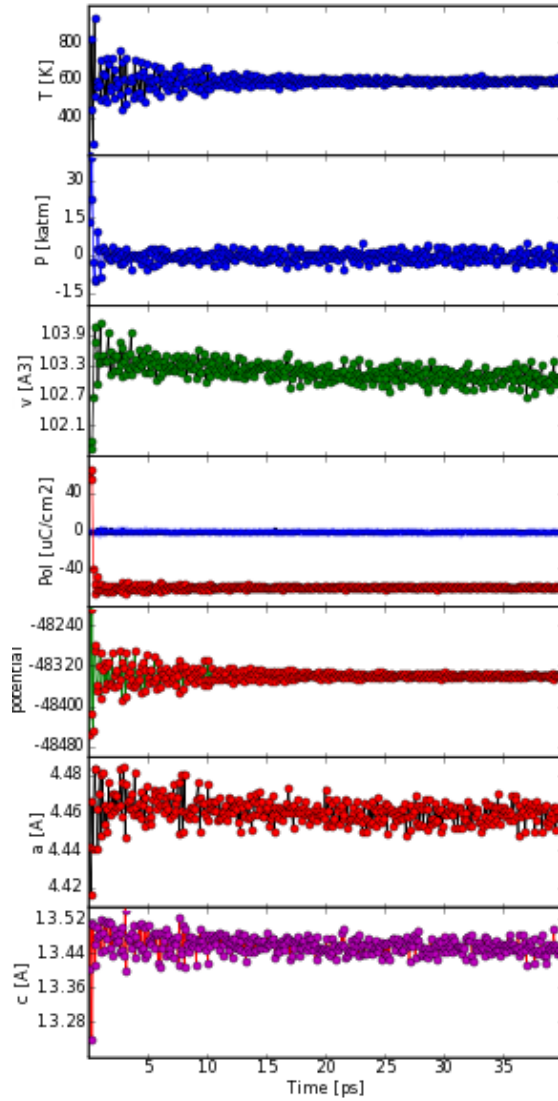


Figure 7: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=600$  K (new20081030).

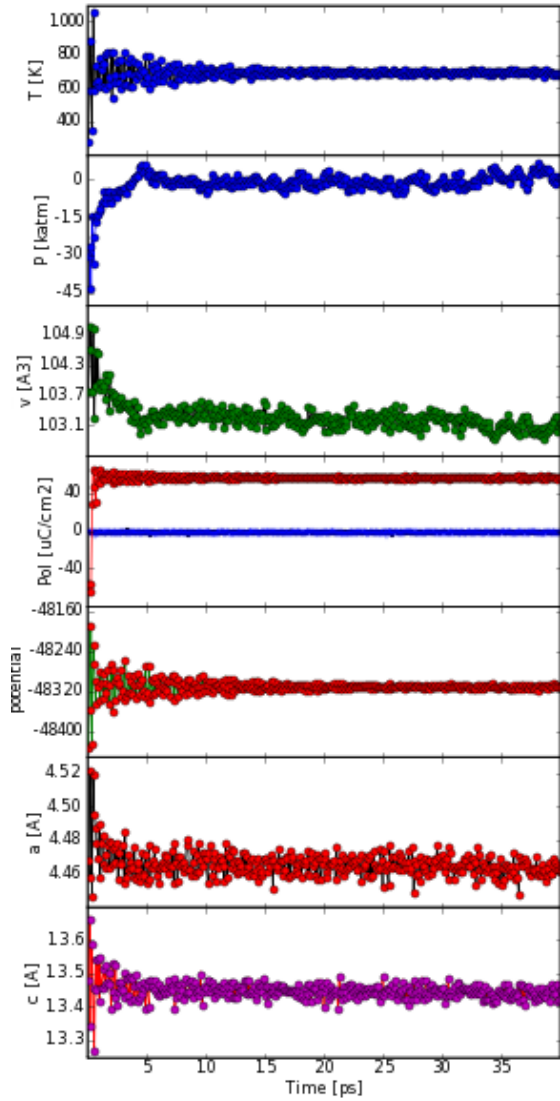


Figure 8: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=700$  K (new20081030).

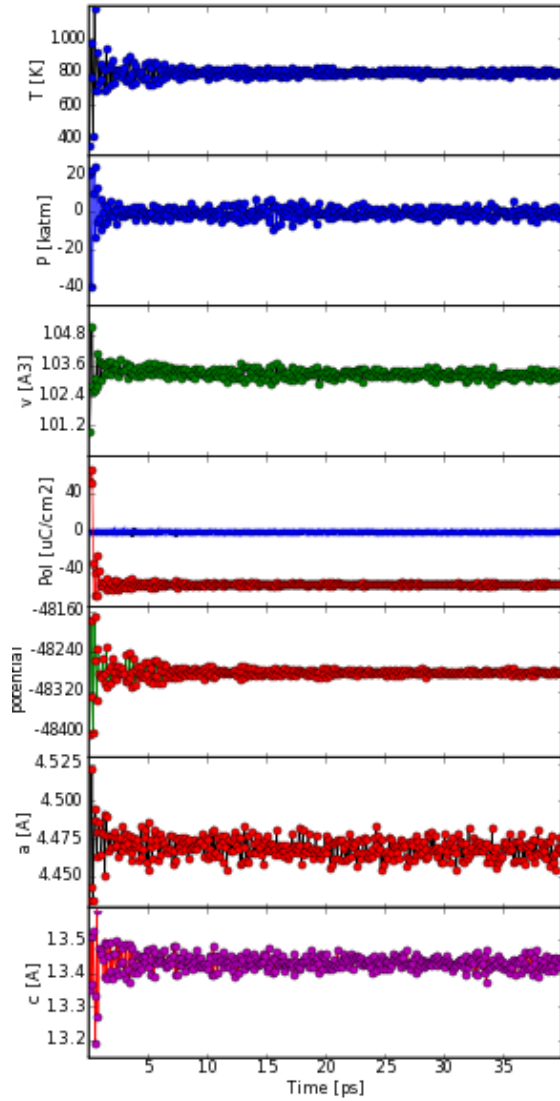


Figure 9: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=800$  K (new20081030).

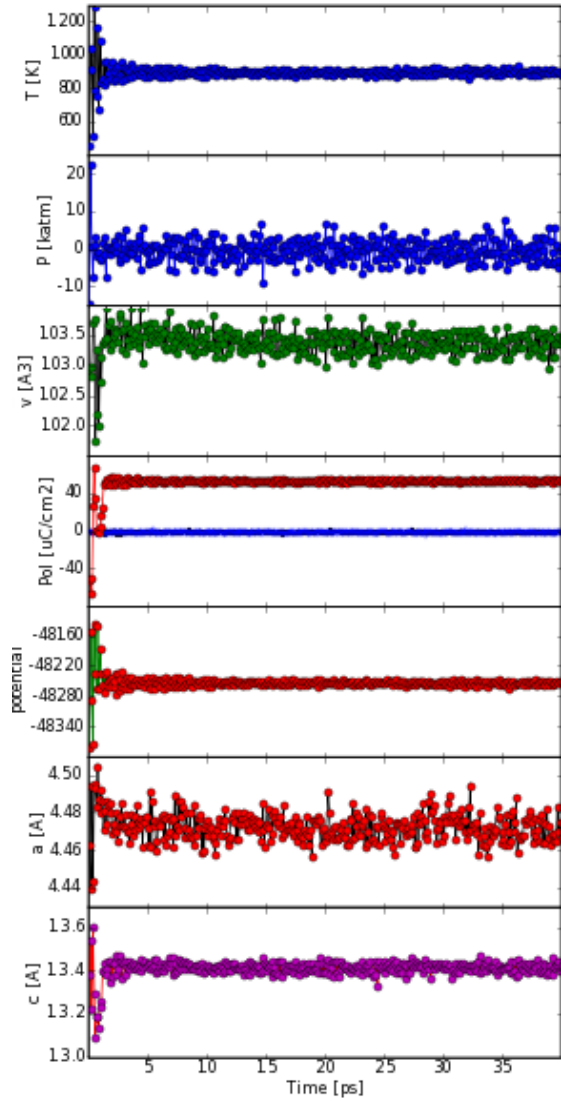


Figure 10: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=900$  K (new20081030).

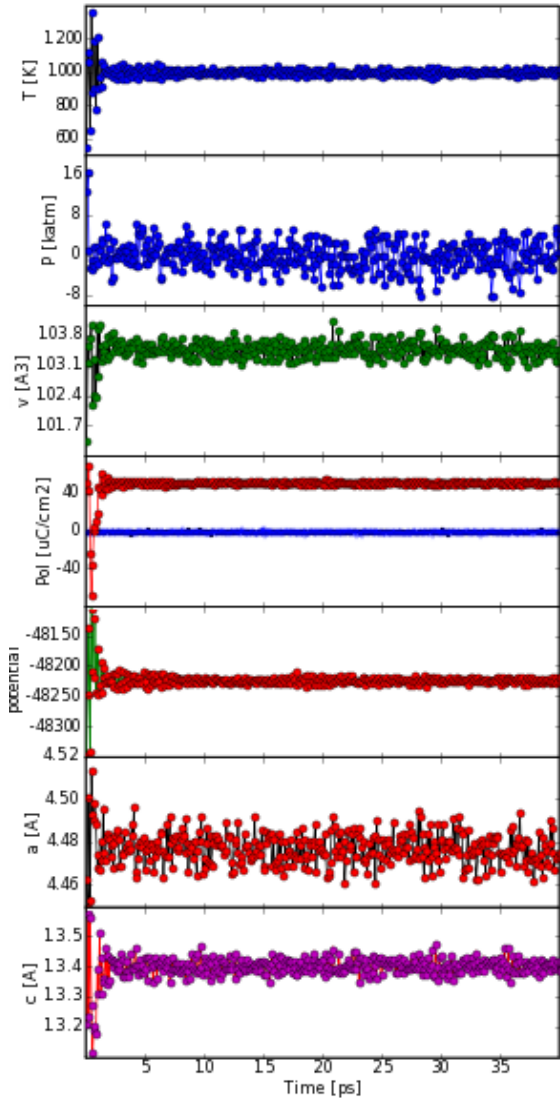


Figure 11: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1000$  K (new20081030).

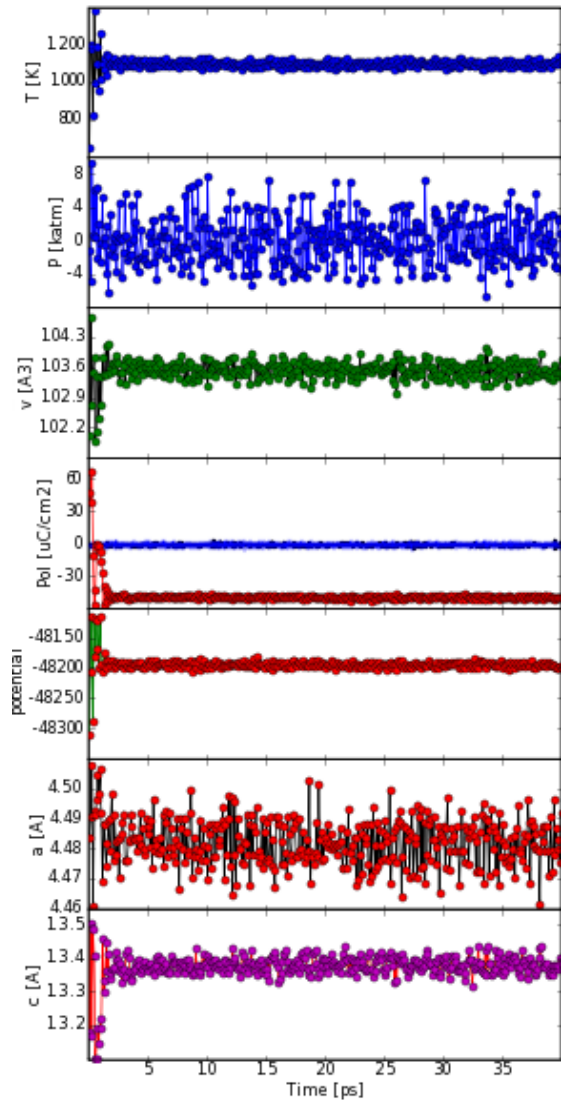


Figure 12: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1100$  K (new20081030).