

# 1 CONTROL

DLPOLY: LiNbO3

```
temperature 1150.000000
pressure 0.000000
steps 200000
equilibration 0
print every 200
stats every 200
timestep 0.0002000000 ps
ensemble nst hoover 0.500000 0.500000 (ps)
traj 1 200 0
rdf 1000
multiple step 1
cap 1000
scale 100
restart scale
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

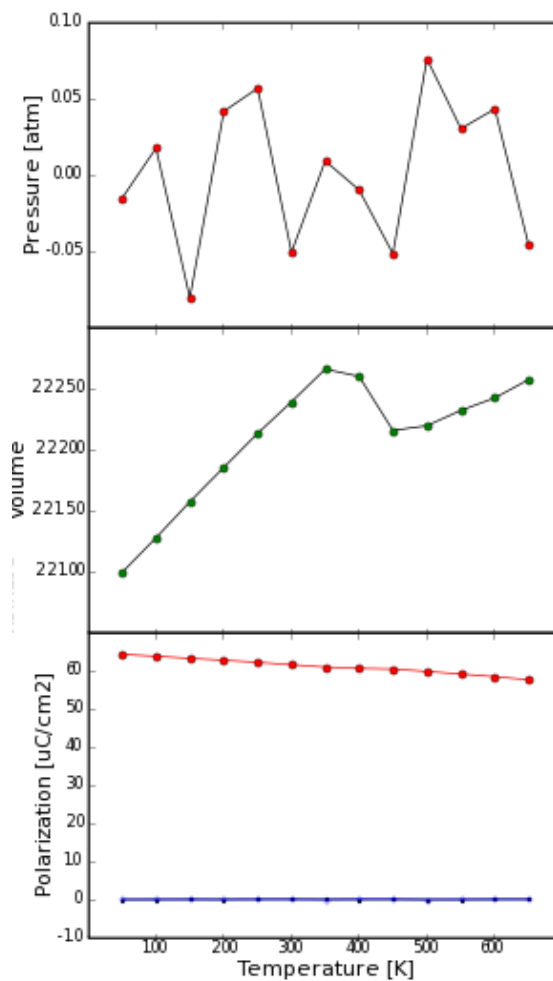


Figure 1: Pressure, Volume, Polarization verse temperature for MD simulation of LiNbO3 (run2008Jan25 -g ).

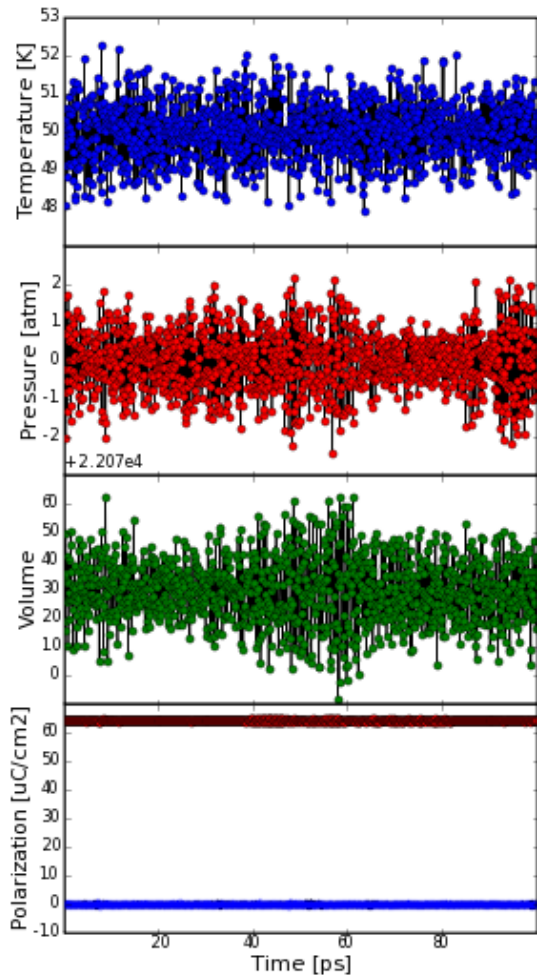


Figure 2: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=50$  K (run2008Jan25).

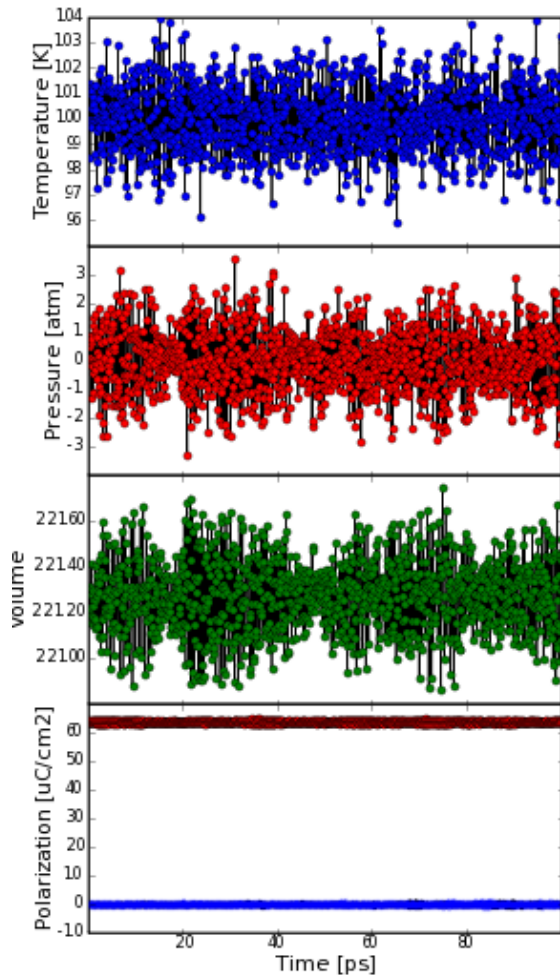


Figure 3: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=100$  K (run2008Jan25).

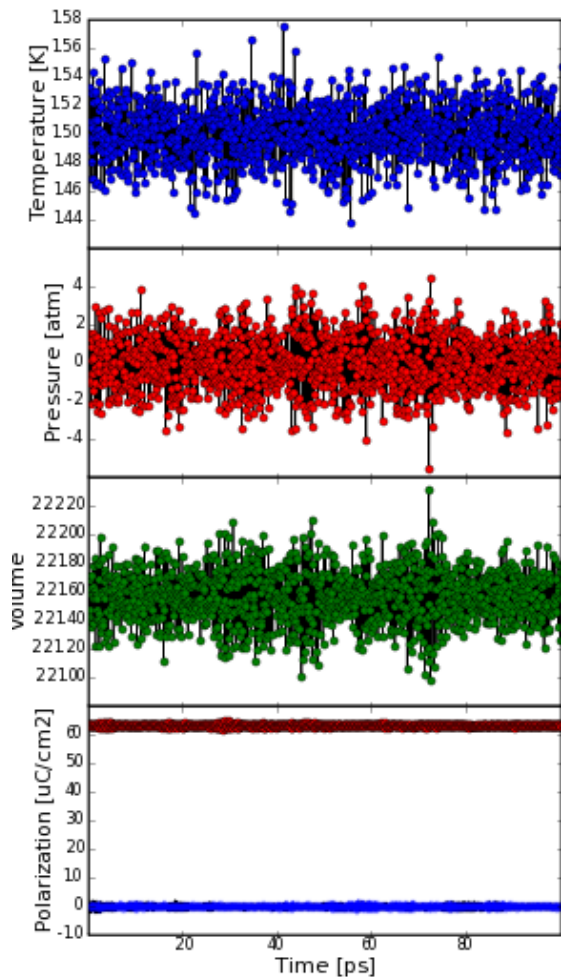


Figure 4: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=150$  K (run2008Jan25).

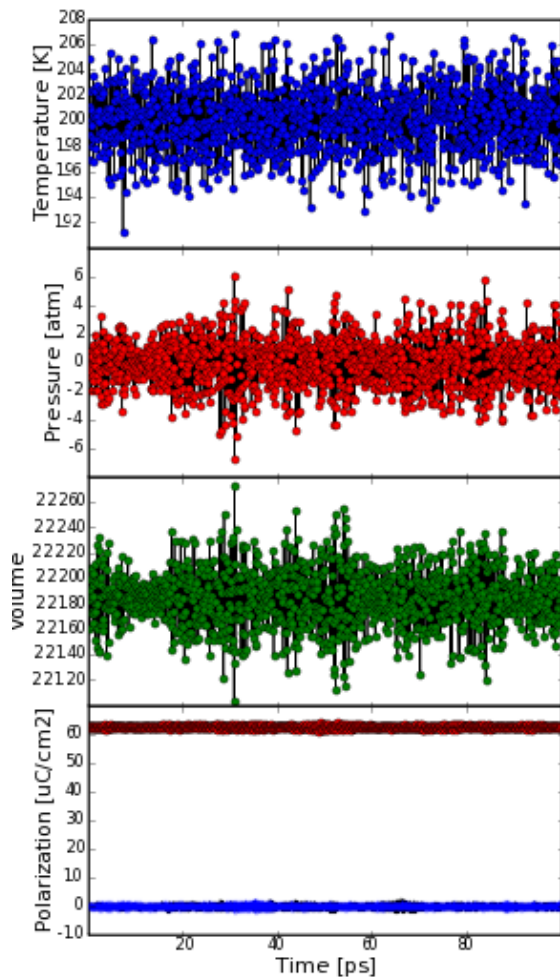


Figure 5: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=200$  K (run2008Jan25).

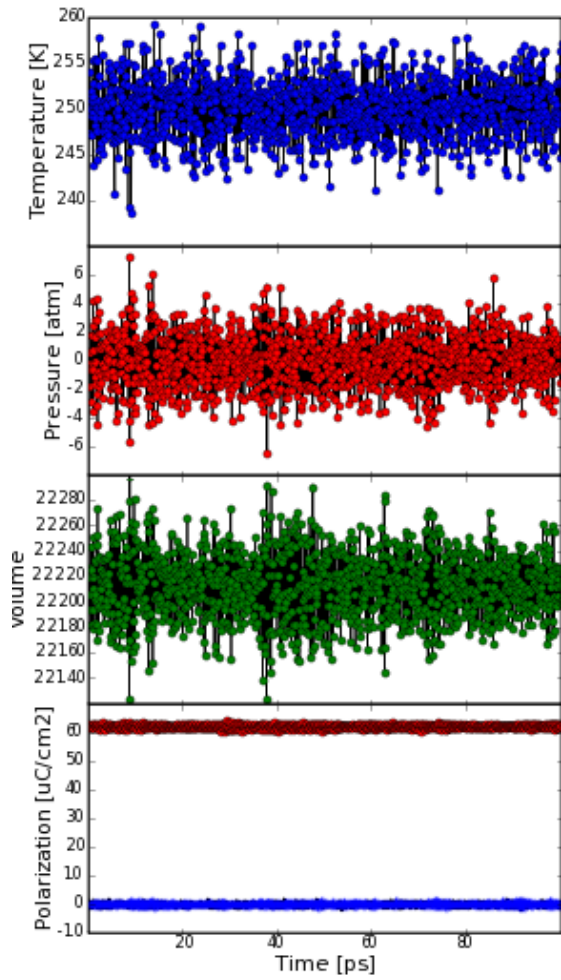


Figure 6: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=250$  K (run2008Jan25).

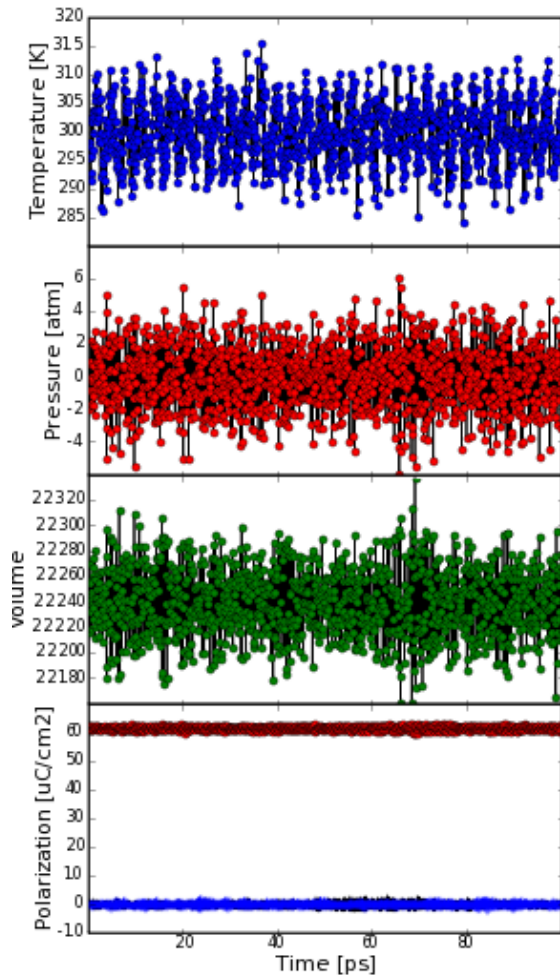


Figure 7: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=300$  K (run2008Jan25).

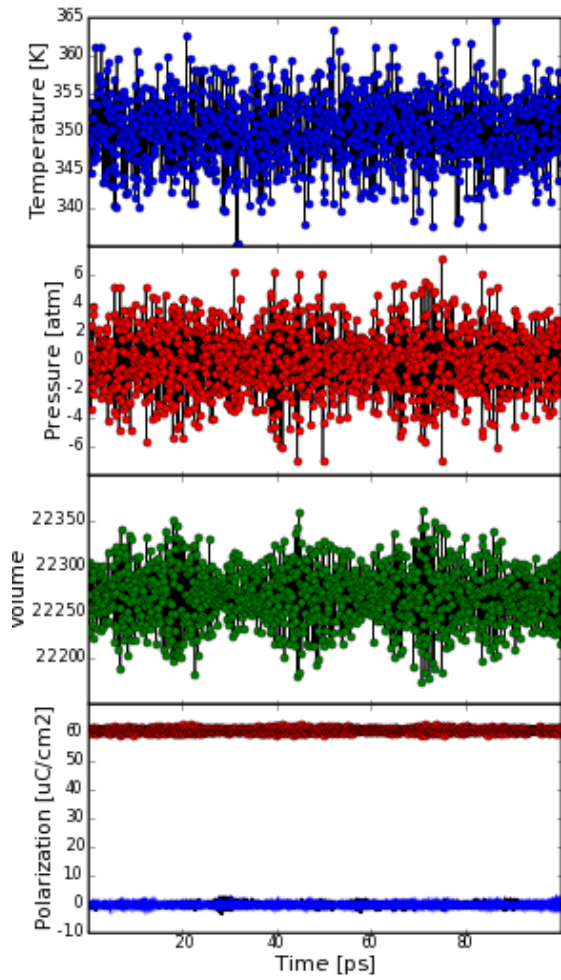


Figure 8: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=350$  K (run2008Jan25).

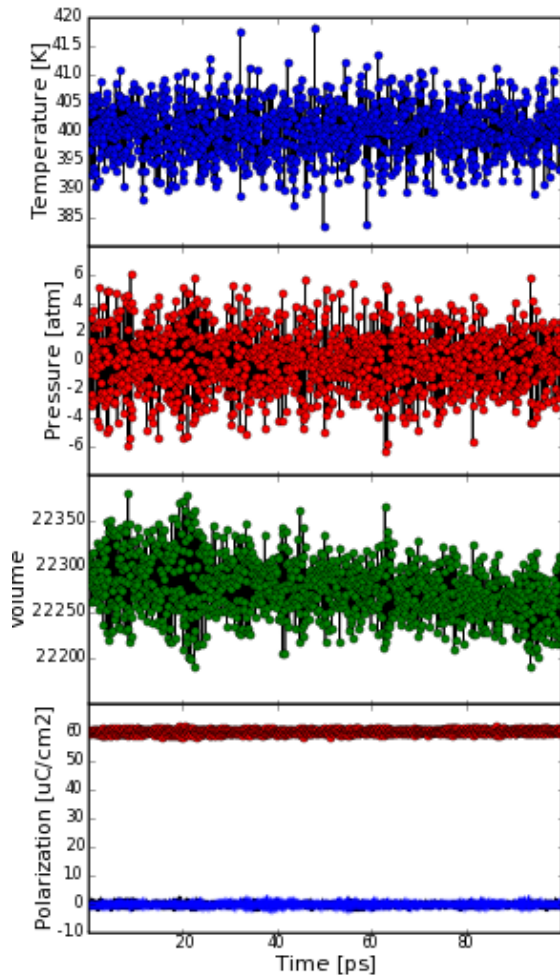


Figure 9: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=400$  K (run2008Jan25).

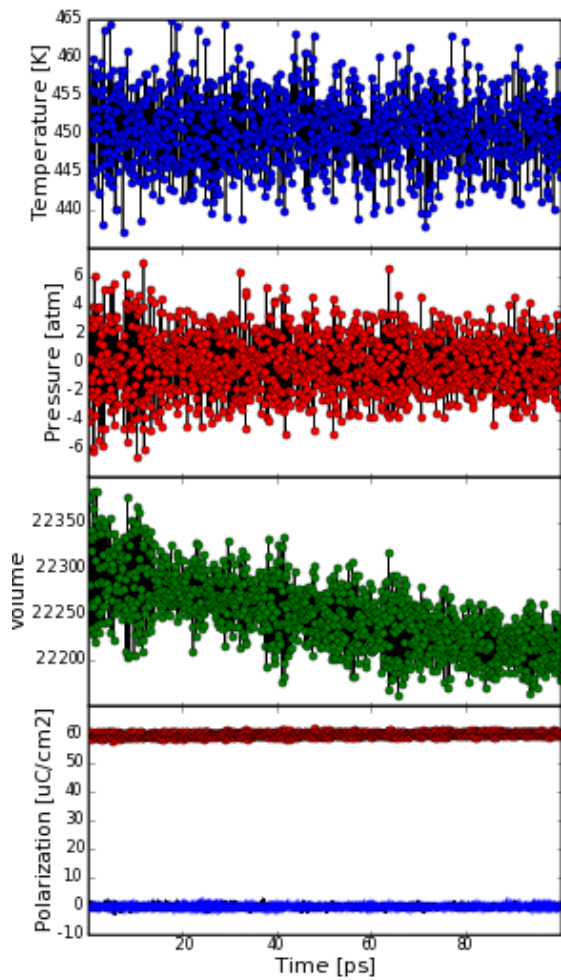


Figure 10: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=450$  K (run2008Jan25).

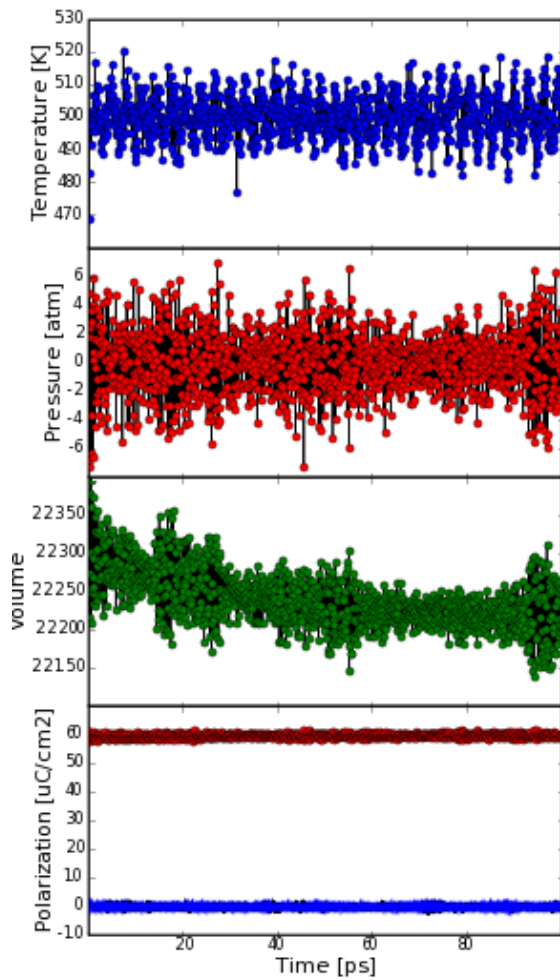


Figure 11: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=500$  K (run2008Jan25).

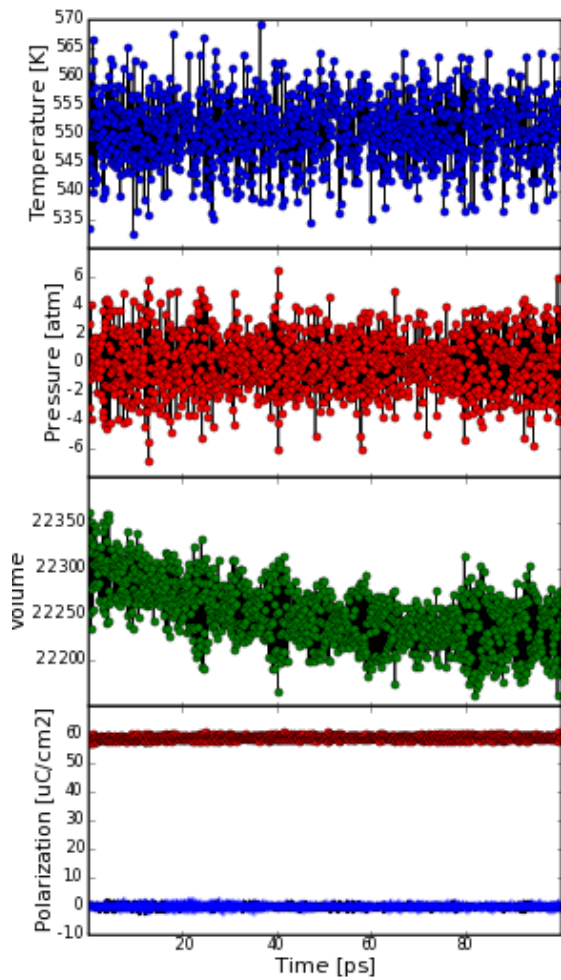


Figure 12: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=550$  K (run2008Jan25).

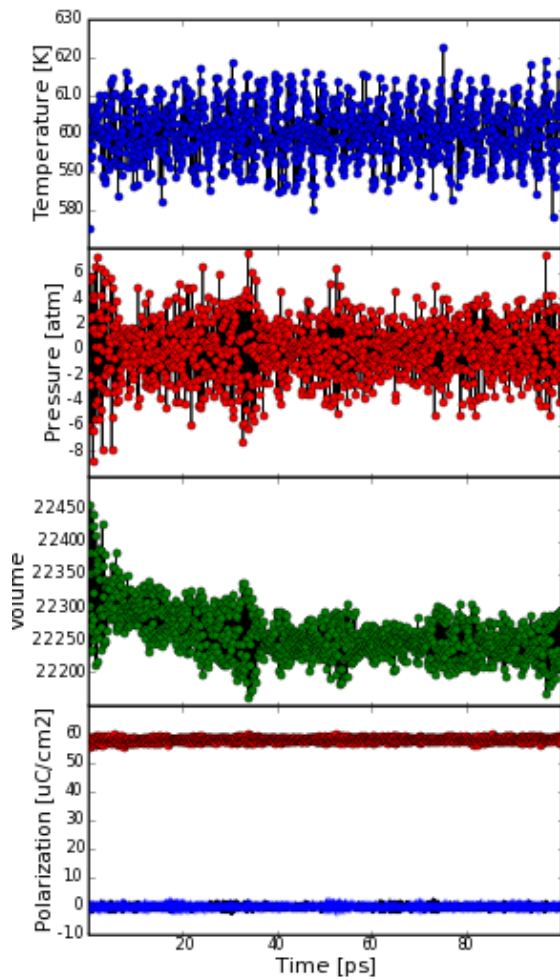


Figure 13: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=600$  K (run2008Jan25).

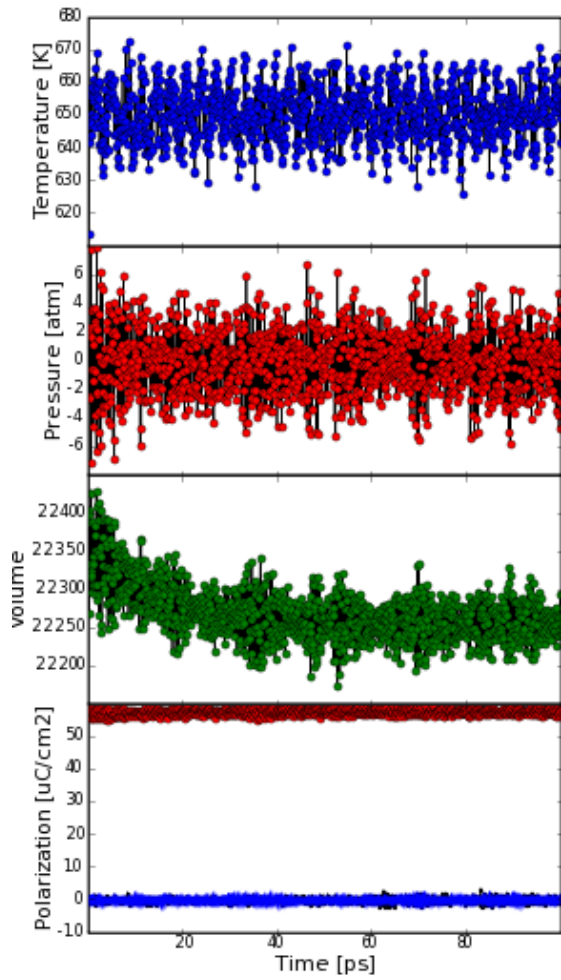


Figure 14: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=650$  K (run2008Jan25).