

1 CONTROL

DLPOLY: LiNbO3

```
temperature 2100.000000
pressure 0.000000
steps 100000
equilibration 20000
print every 500
stats every 500
timestep 0.0004000000 ps
ensemble nst hoover 0.600000 0.500000 (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

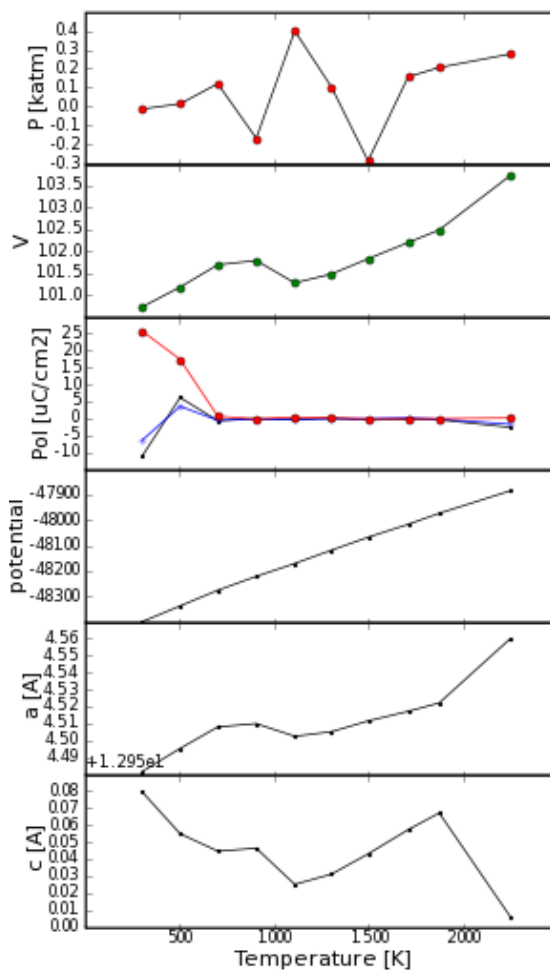


Figure 1: Pressure, Volume, Polarization verse temperature for MD simulation of LiNbO3 (LNO2009Nov7 -d).

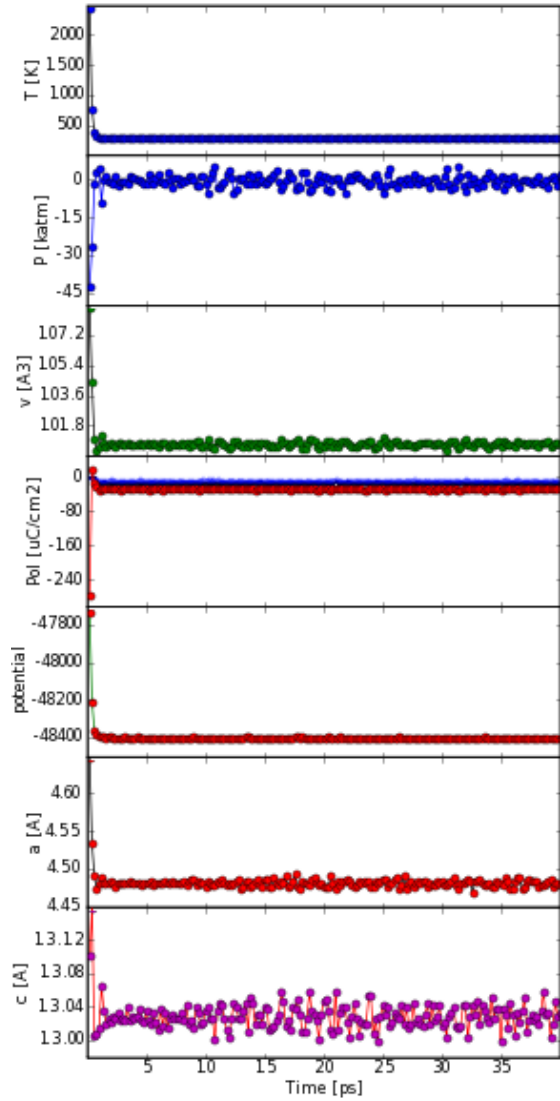


Figure 2: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=300$ K (LNO2009Nov7).

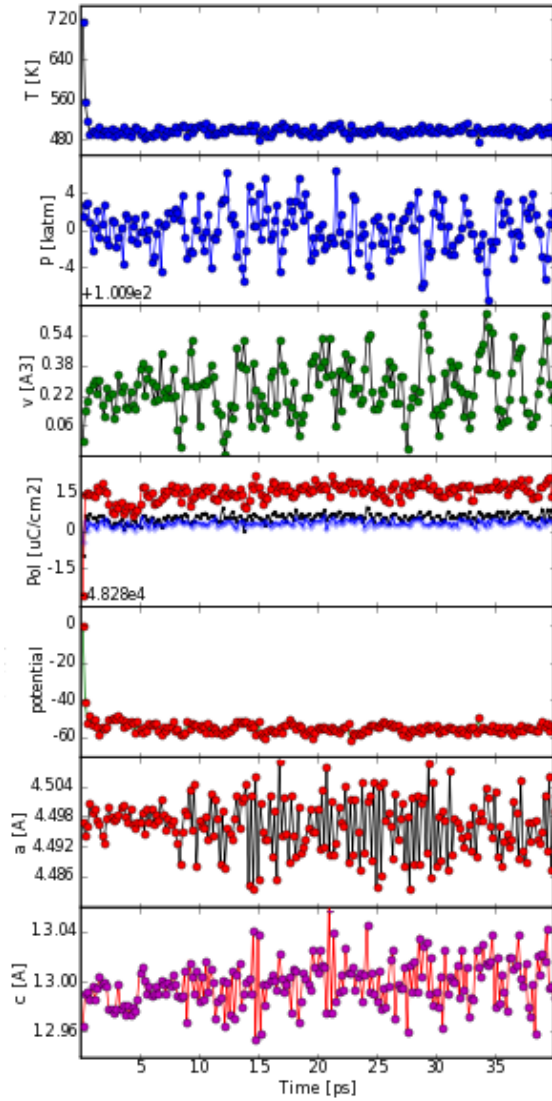


Figure 3: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=500$ K (LNO2009Nov7).

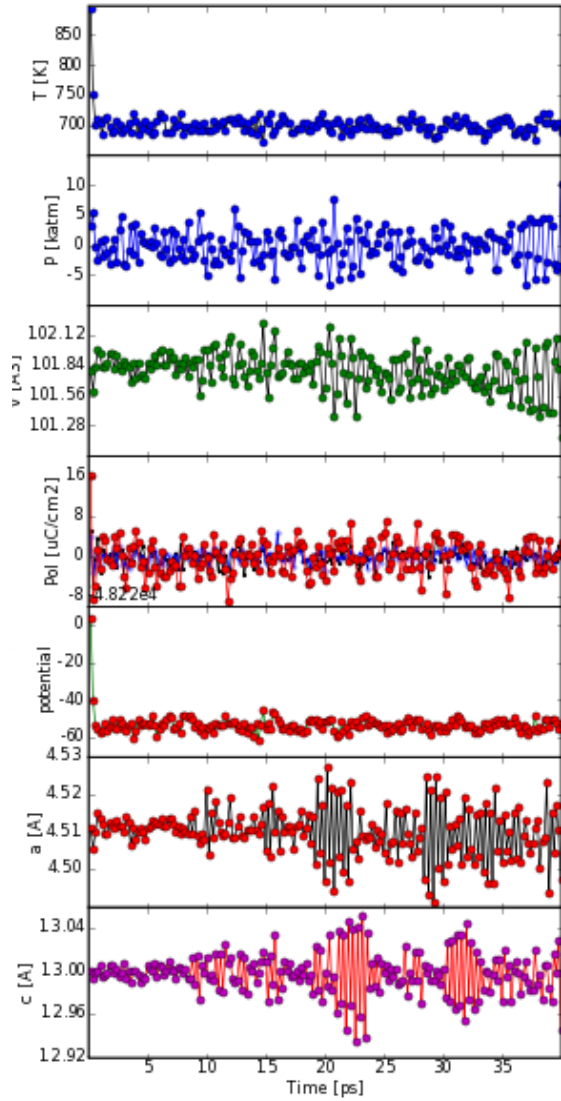


Figure 4: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=700$ K (LNO2009Nov7).

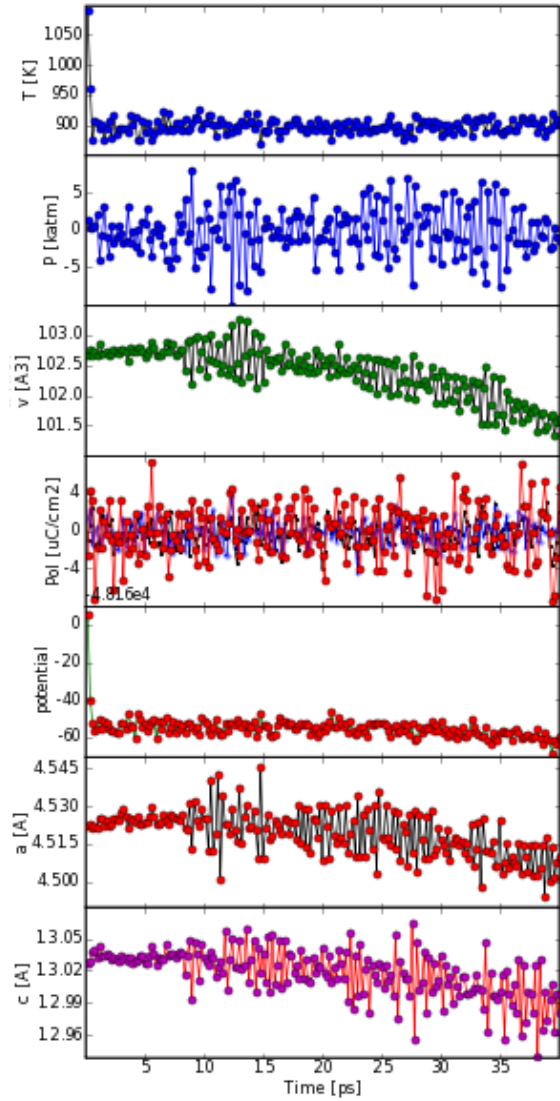


Figure 5: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=900$ K (LNO2009Nov7).

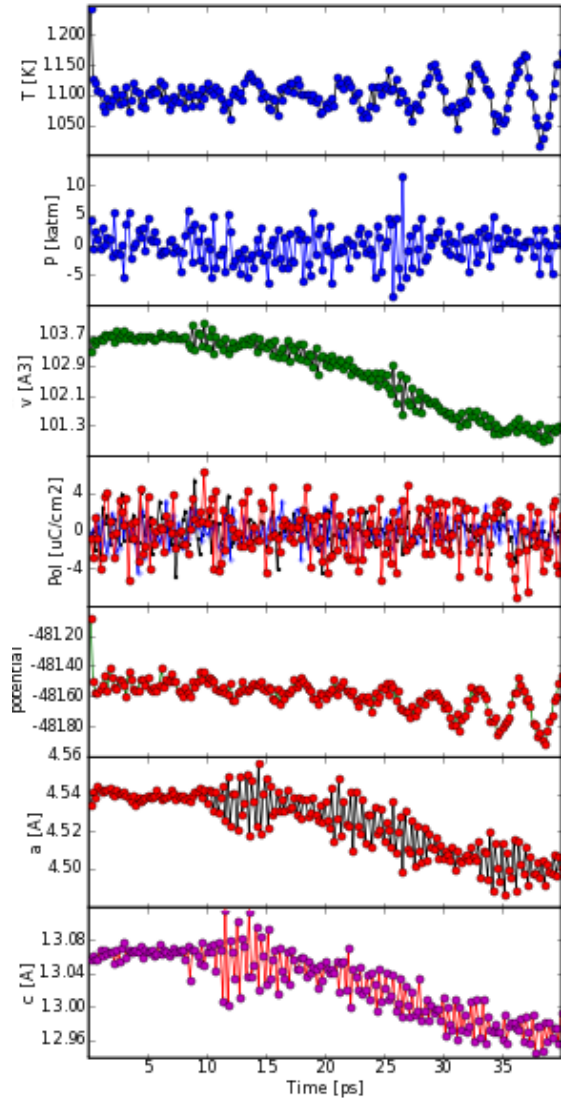


Figure 6: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1100$ K (LNO2009Nov7).

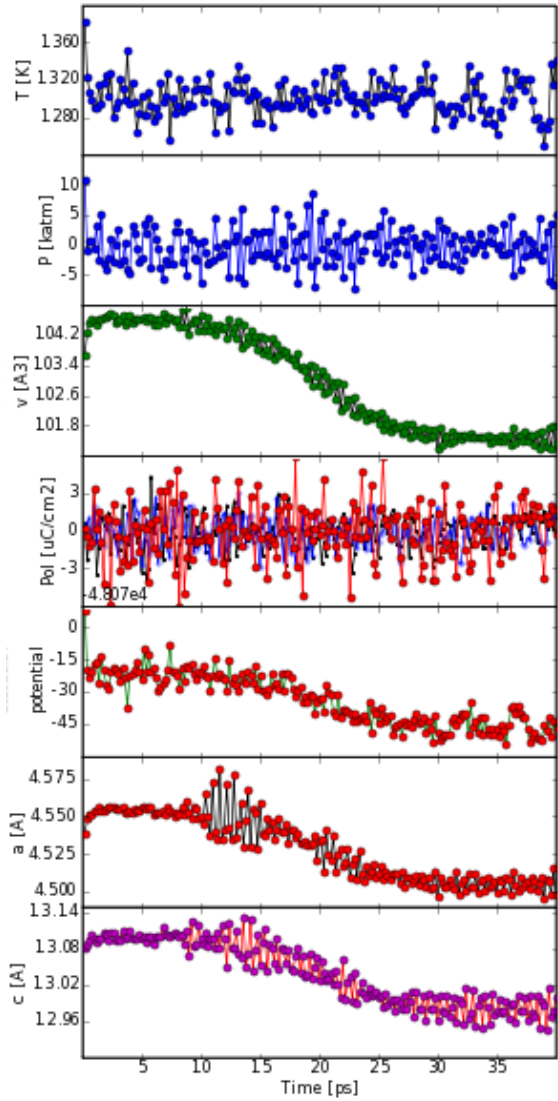


Figure 7: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1300$ K (LNO2009Nov7).

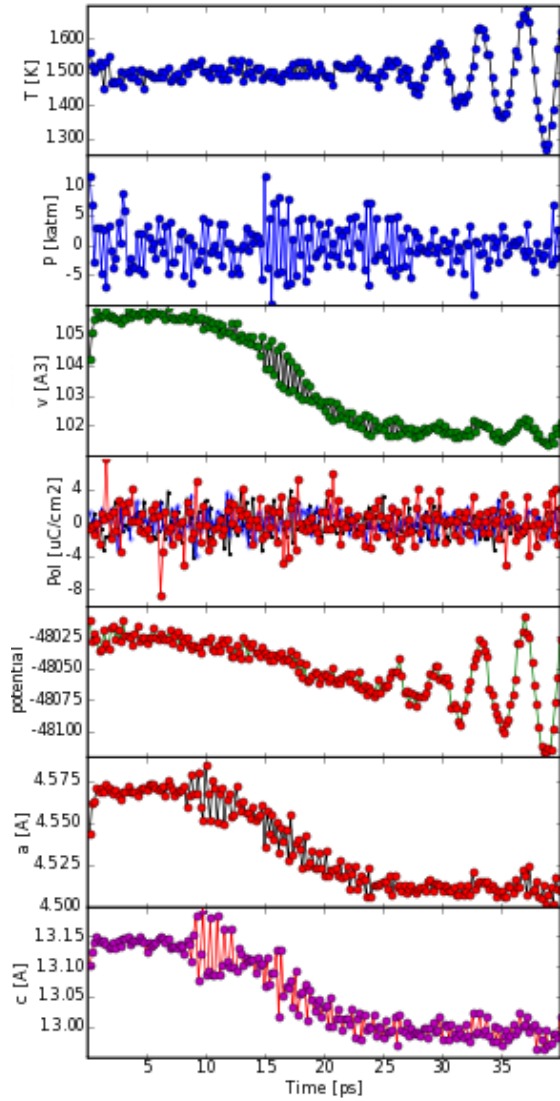


Figure 8: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1500$ K (LNO2009Nov7).

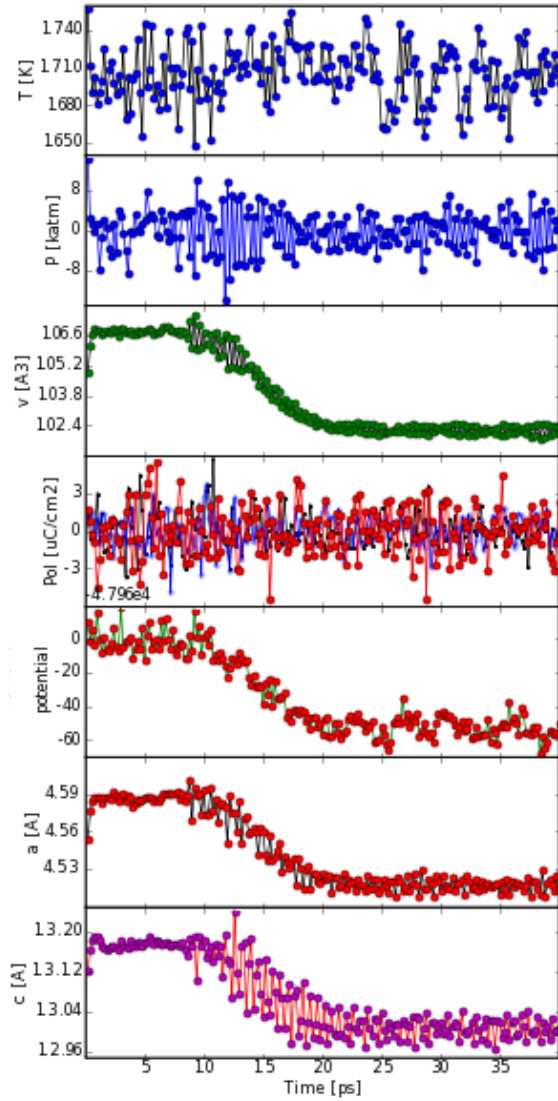


Figure 9: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1700$ K (LNO2009Nov7).

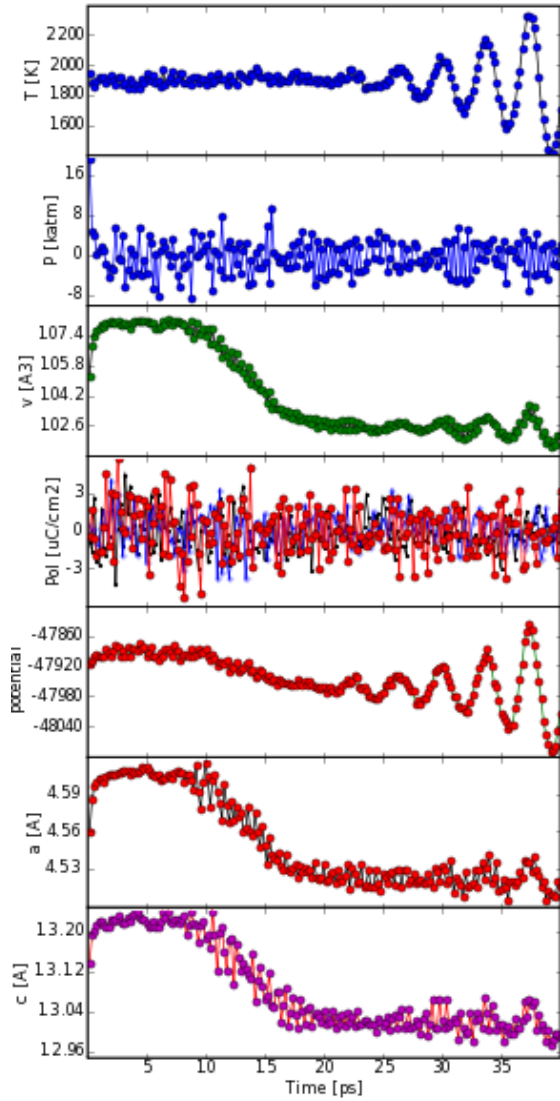


Figure 10: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1900$ K (LNO2009Nov7).

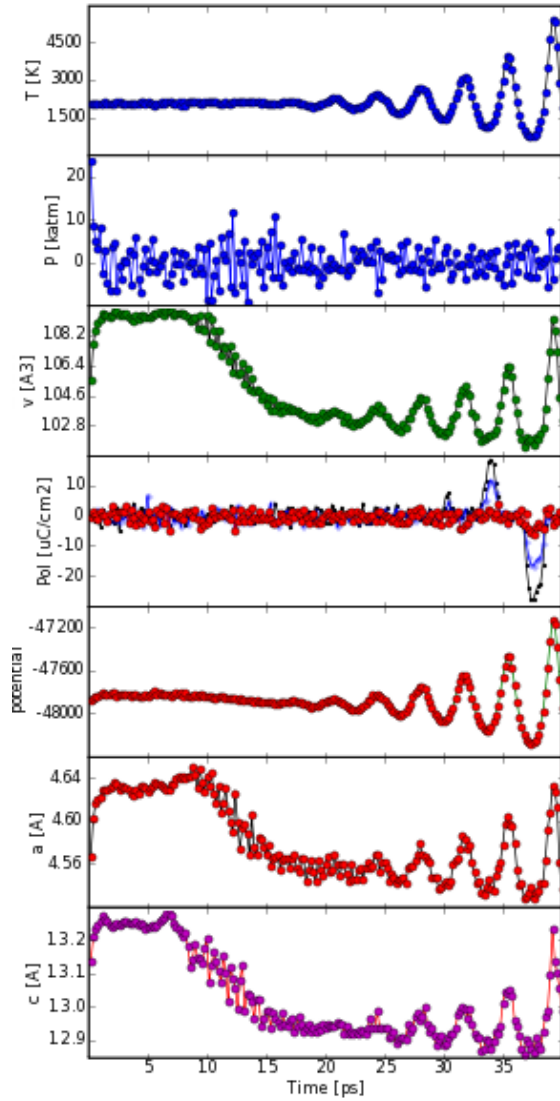


Figure 11: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=2100$ K (LNO2009Nov7).