

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 0.200000 0.600000 (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

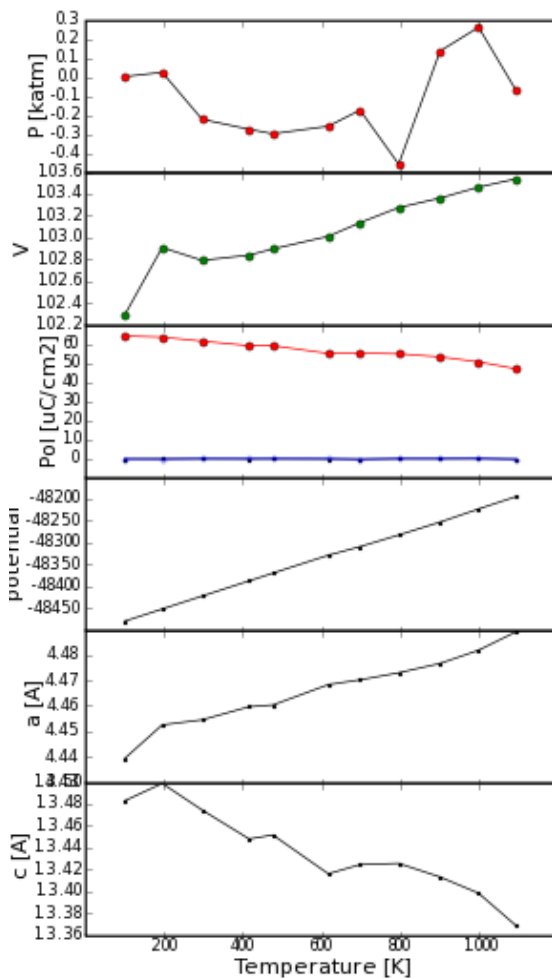


Figure 1: Pressure, Volume, Polarization verse temperature for MD simulation of LiNbO3 (new20081027 -c).

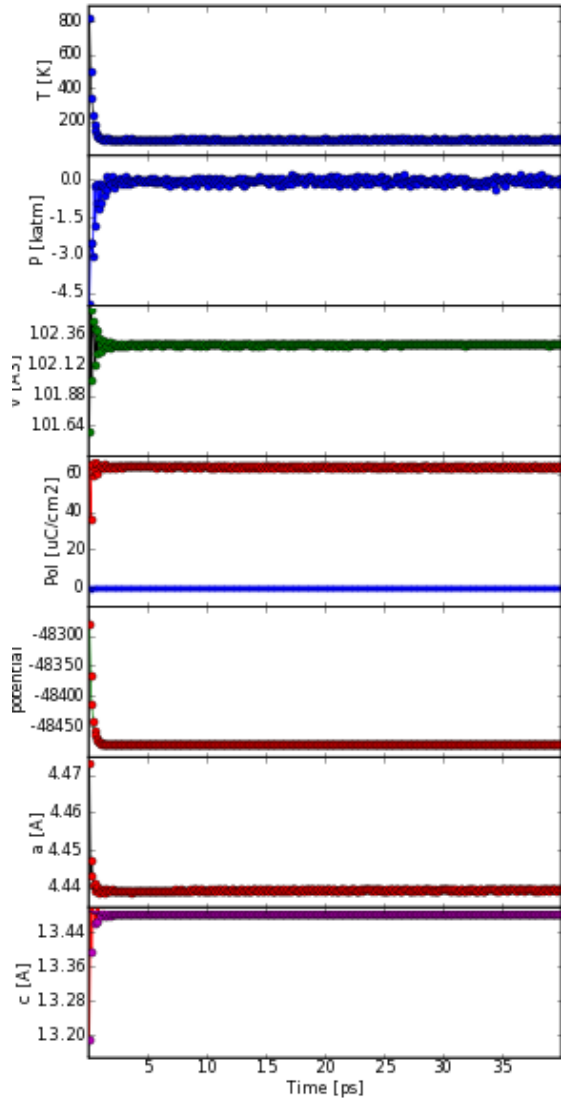


Figure 2: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=100$ K (new20081027).

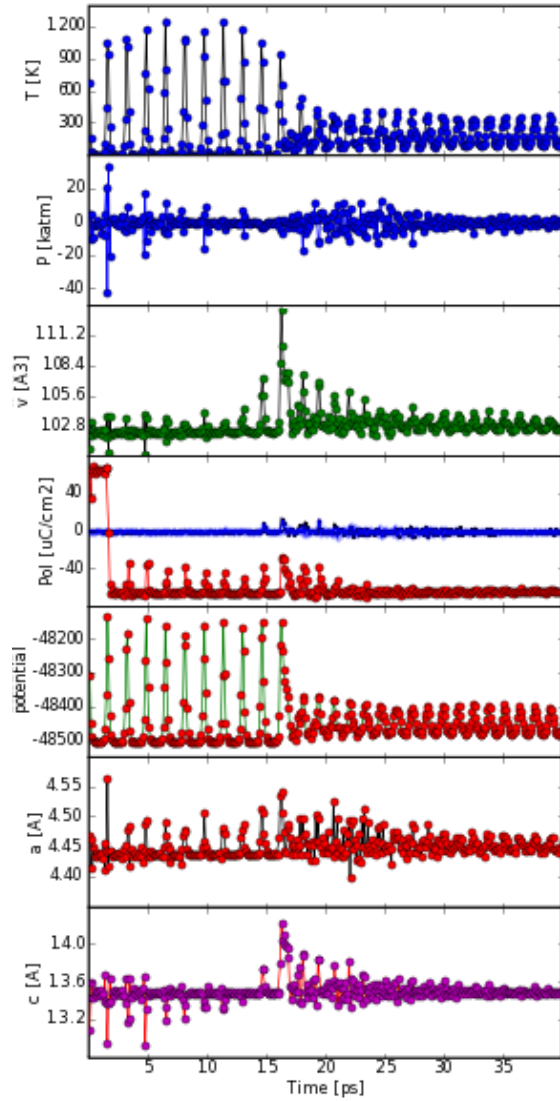


Figure 3: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=200$ K (new20081027).

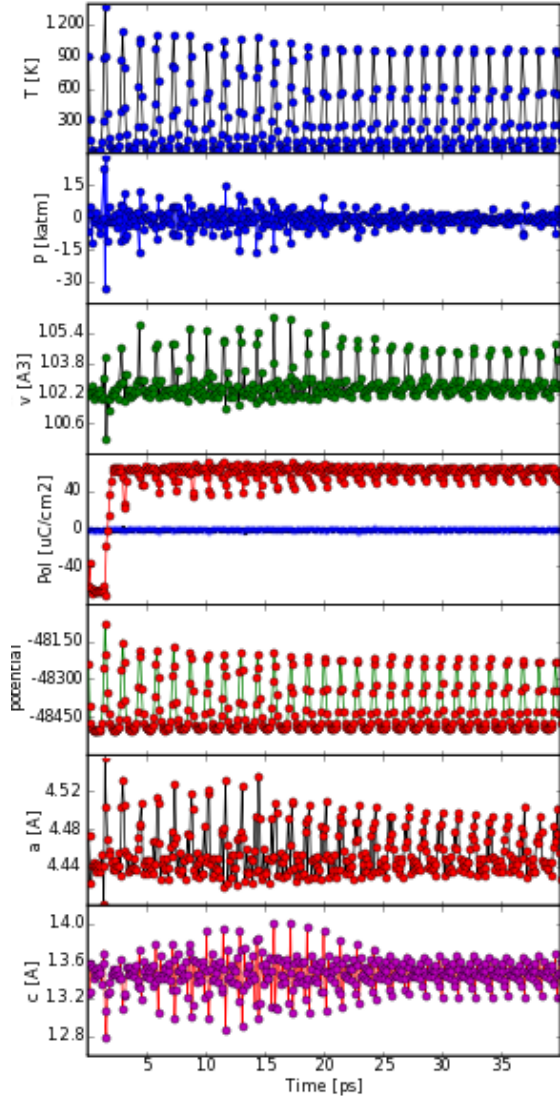


Figure 4: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=300$ K (new20081027).

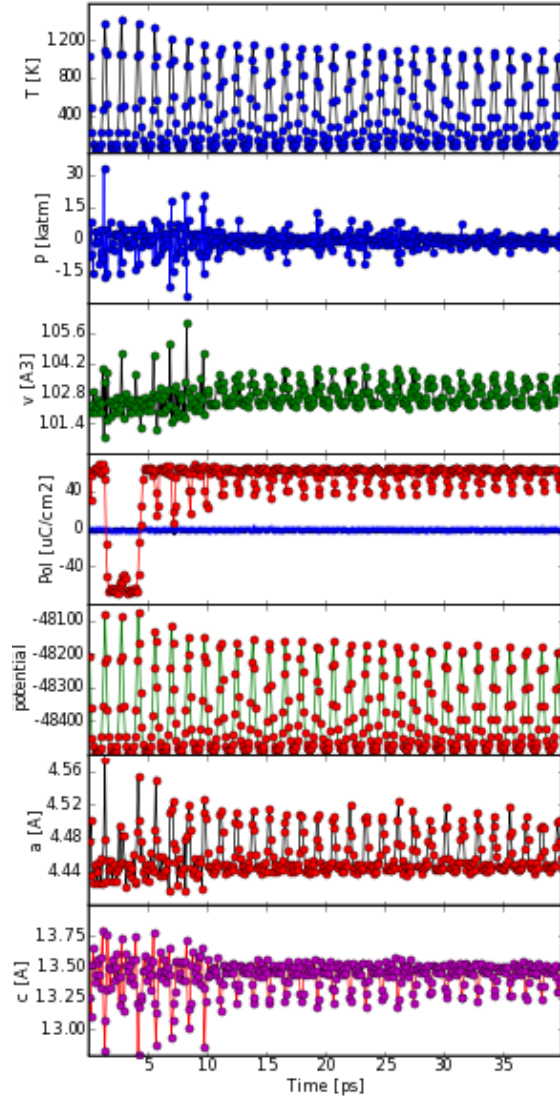


Figure 5: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=400$ K (new20081027).

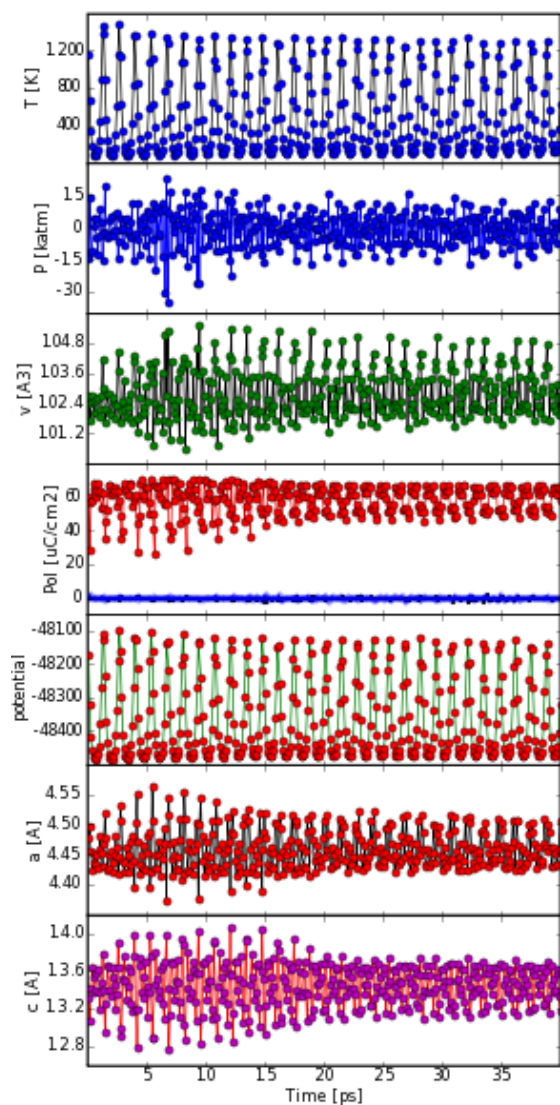


Figure 6: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=500$ K (new20081027).

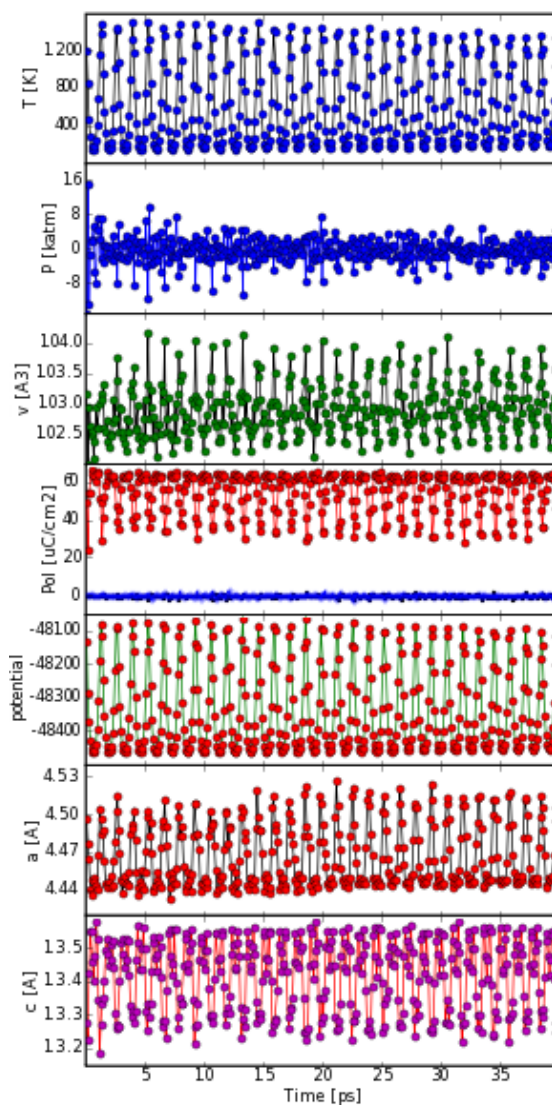


Figure 7: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=600$ K (new20081027).

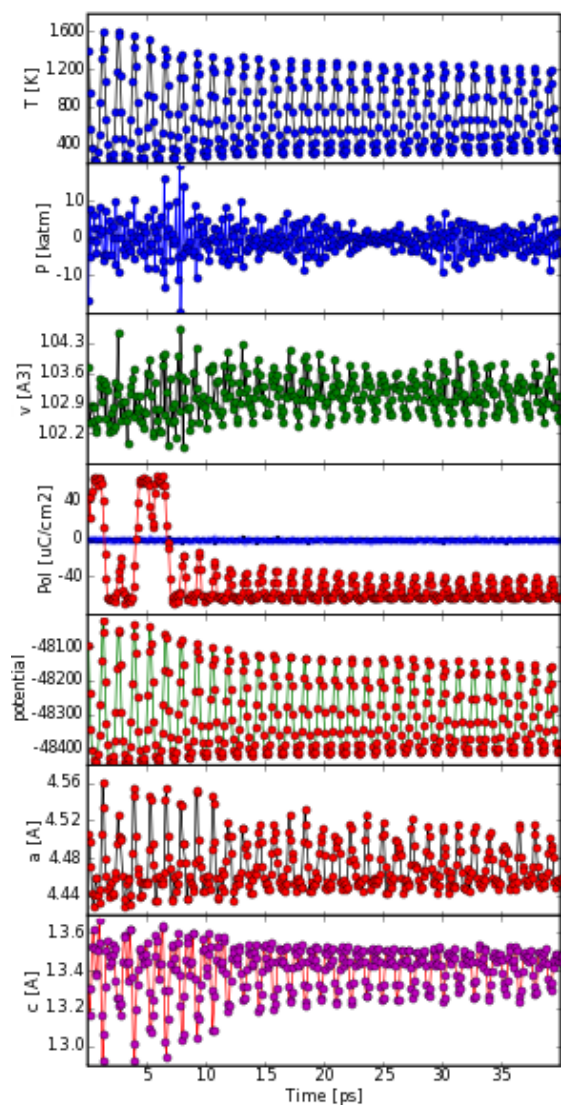


Figure 8: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=700$ K (new20081027).

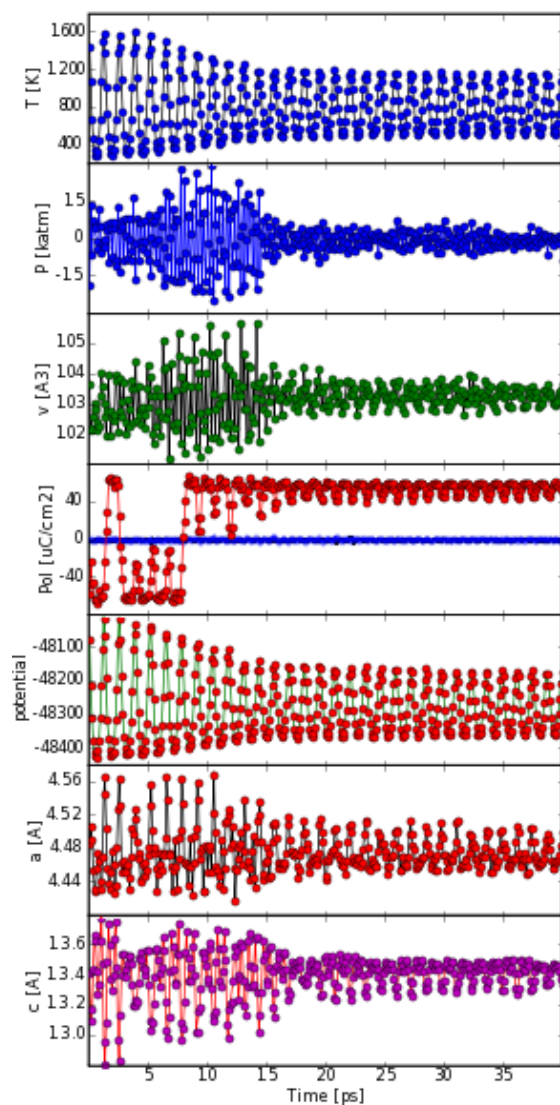


Figure 9: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=800$ K (new20081027).

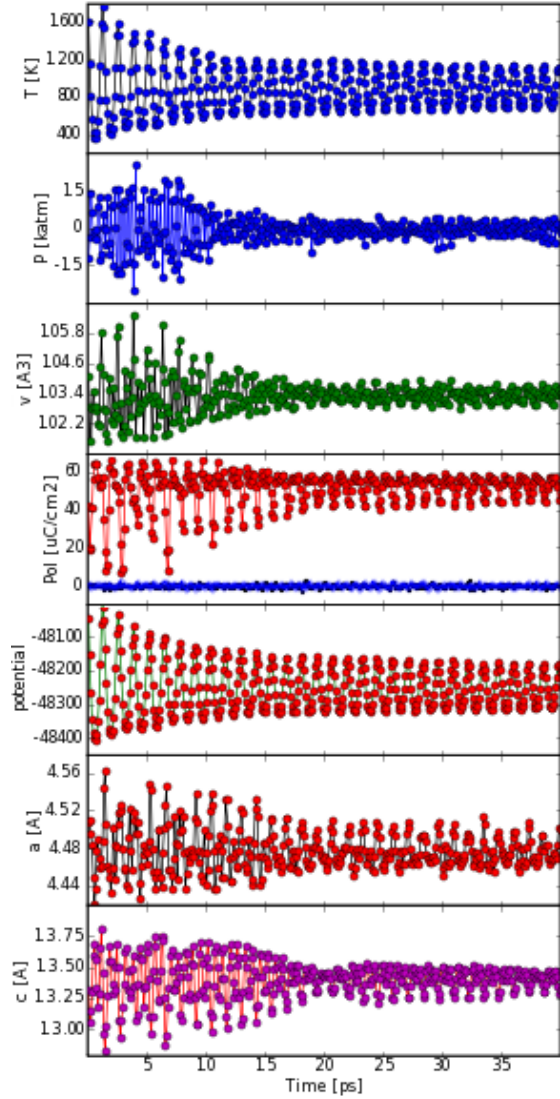


Figure 10: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=900$ K (new20081027).

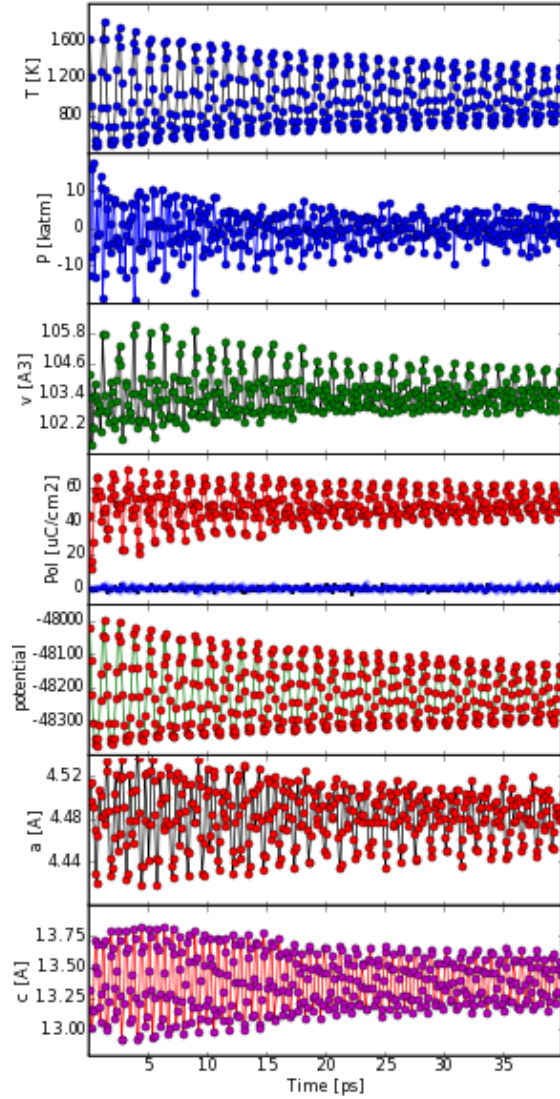


Figure 11: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1000$ K (new20081027).

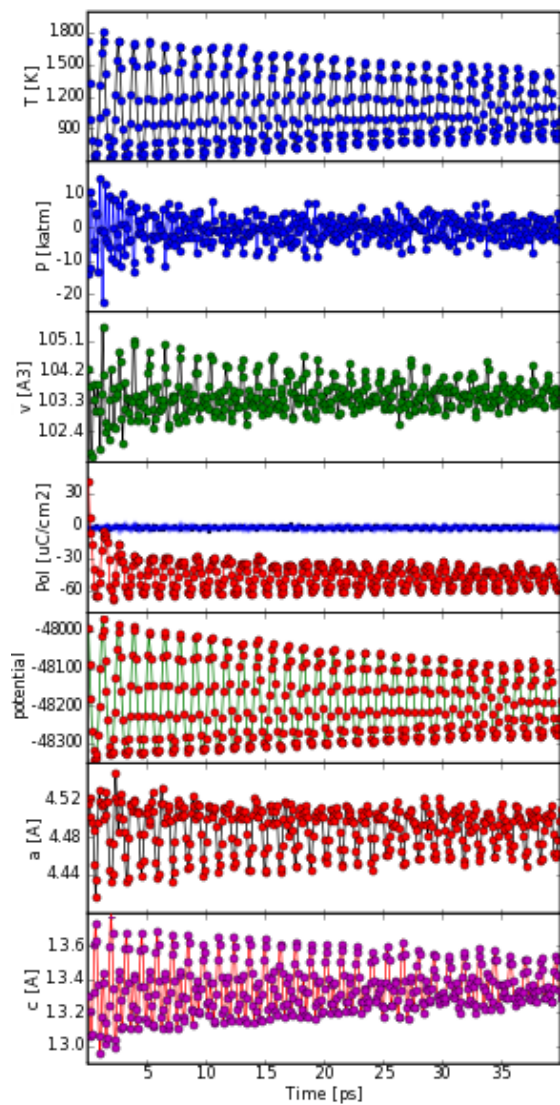


Figure 12: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1100$ K (new20081027).