1 CONTROL

DLPOLY: LiNbO3
temperature 800.000000
pressure 0.000000
steps 200000
equilibration 0
print every 500
stats every 500
timestep 0.0002000000 ps
ensemble nst hoover 0.500000 1.900000 (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

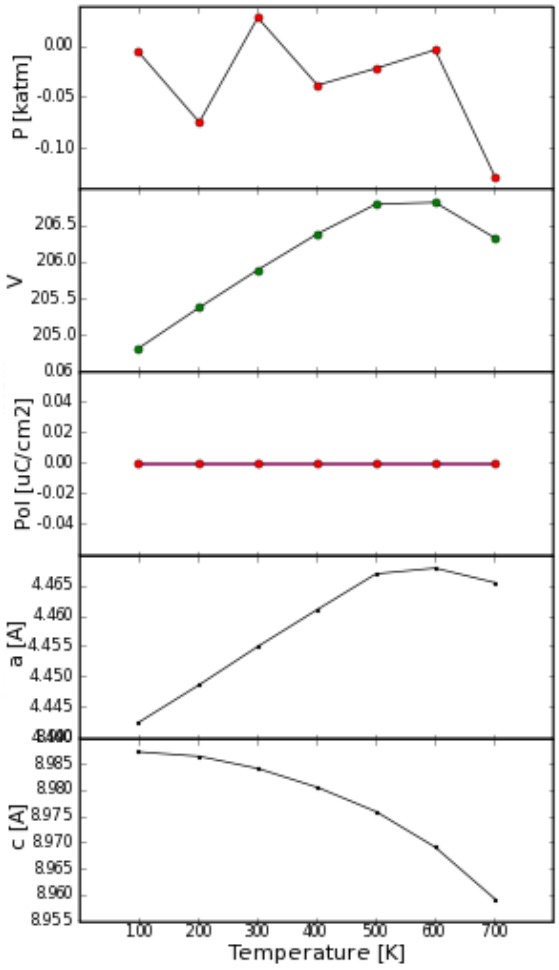

Figure 1: Pressure, Volume, Polarization verse temperature for MD simulation of LiNbO3 (new080824a -c).

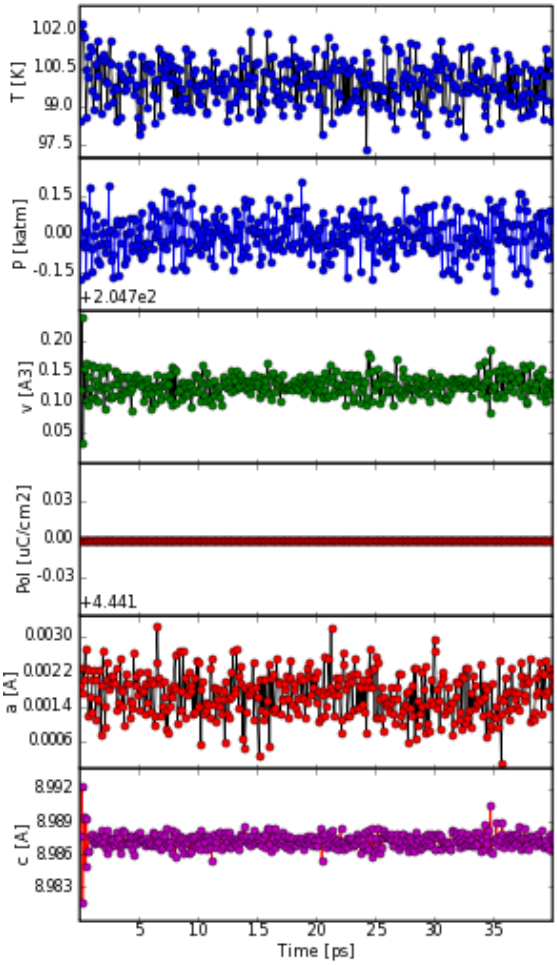

Figure 2: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=100 K (new080824a).

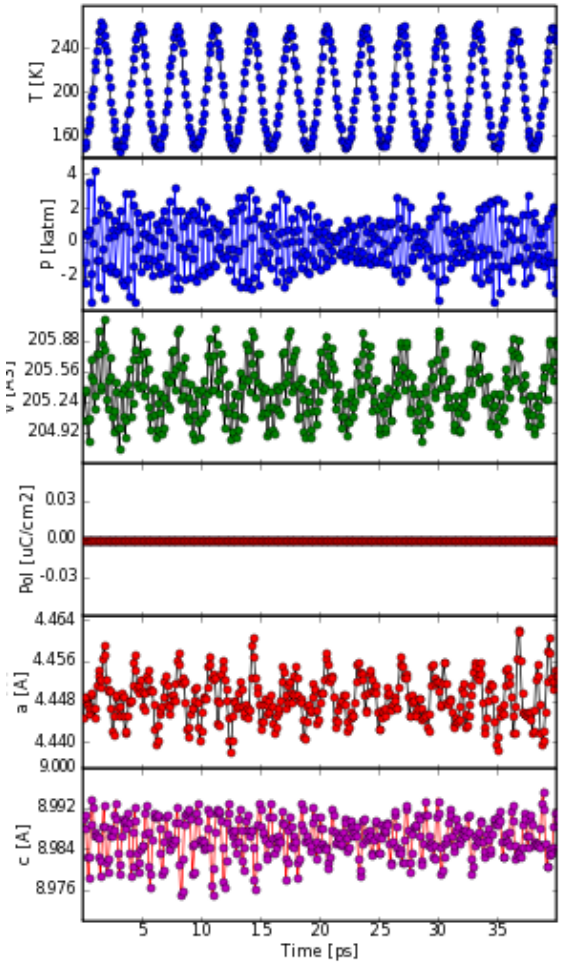

Figure 3: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=200 K (new080824a).

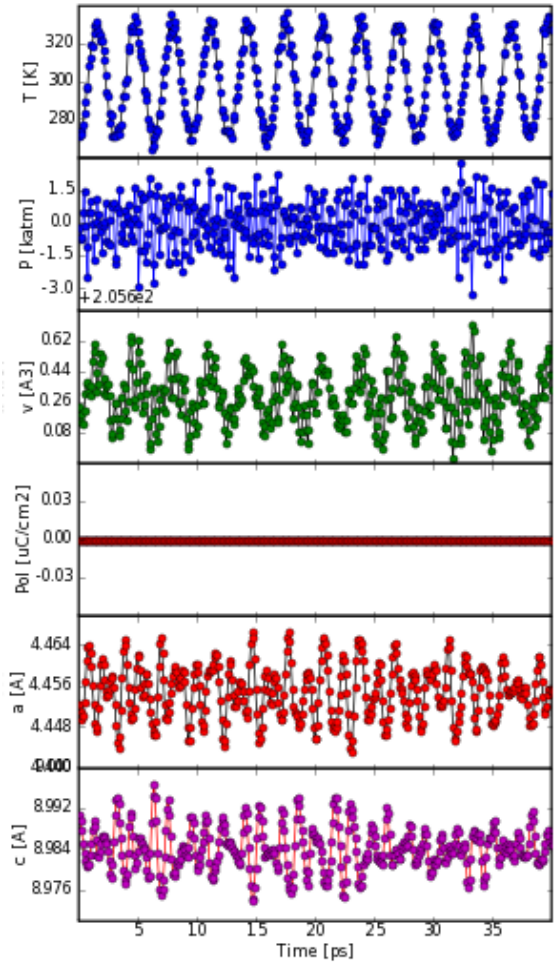

Figure 4: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=300 K (new080824a).

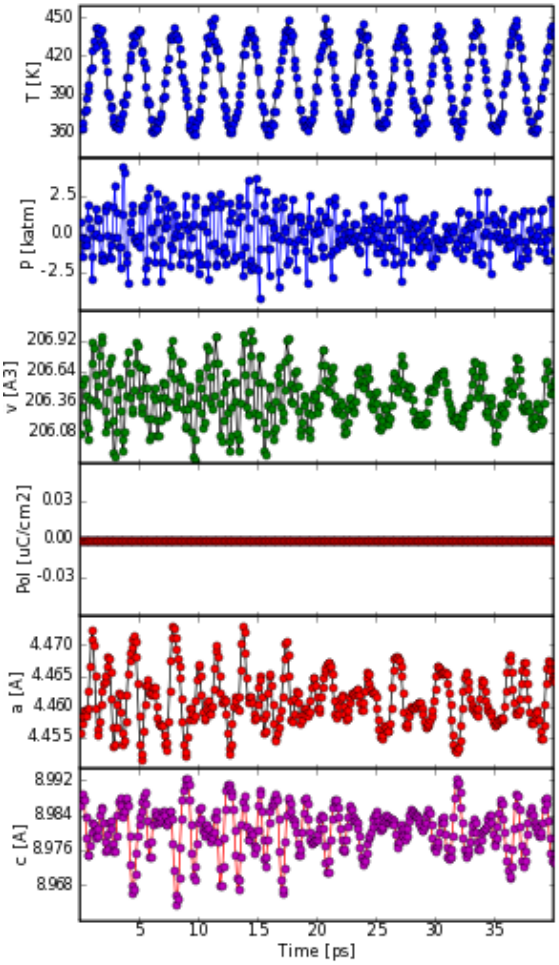

Figure 5: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=400 K (new080824a).

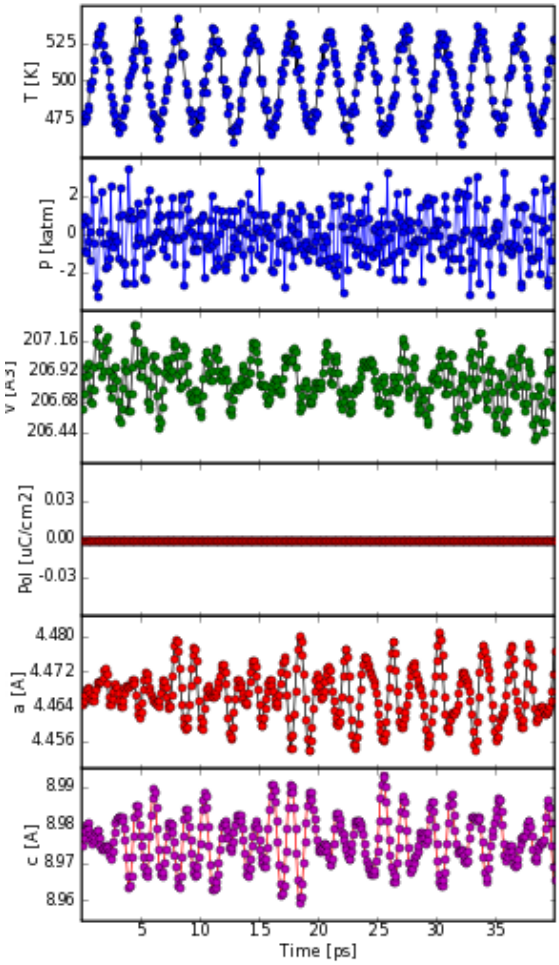

Figure 6: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=500 K (new080824a).

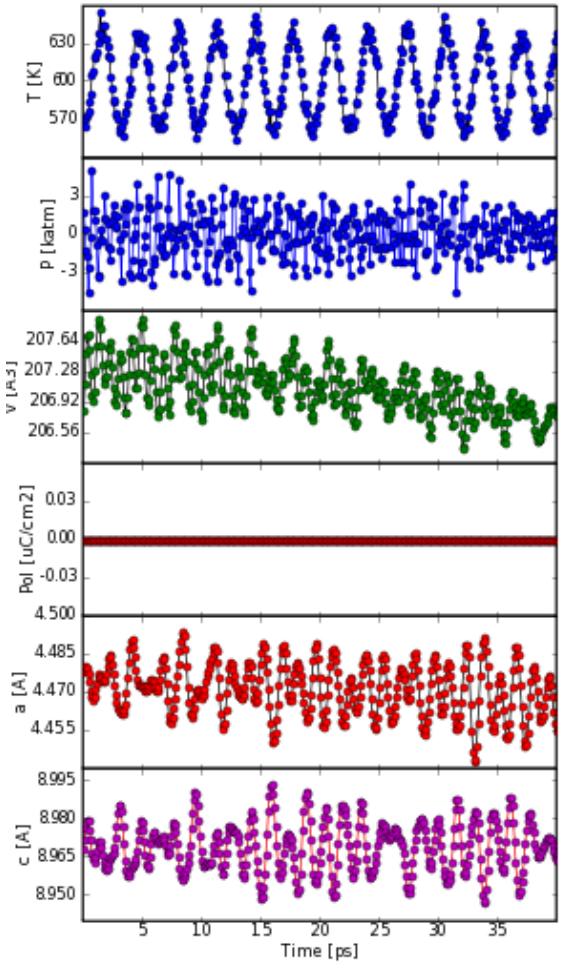

Figure 7: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=600 K (new080824a).

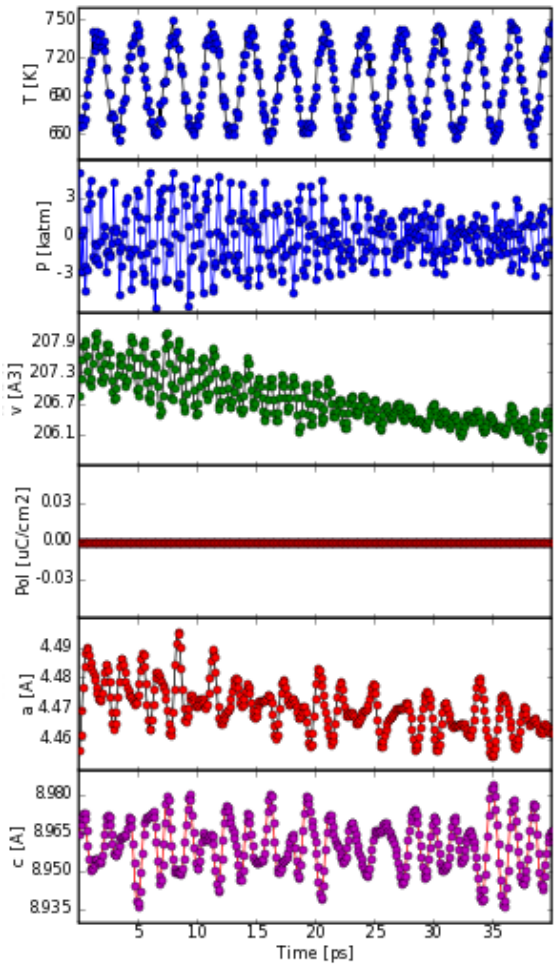

Figure 8: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=700 K (new080824a).