Phonons of $SrTiO_3$ (using phonopy)

- This exercise should be done WITHOUT w2web in a terminal window !
- mkdir SrTiO3; cd SrTiO3;
- makestruct
  - *$SrTiO_3$: SG 221(P m-3m), a=b=c=7.38 bohr, α=β=γ=90°*
  - *Sr (0.5, 0.5, 0.5), Ti (0, 0, 0), O (0.5, 0 , 0)*
  - *setrmt 3%*
- cp init.struct SrTiO3.struct
- init_lapw -b -numk 10 -rkmax 6 # (batch mode)
- phonopy --wien2k -c SrTiO3.struct -d --dim="2 2 2"
- mkdir 1; mkdir 2; mkdir 3
- Copy SrTiO3.structS-001, SrTiO3.structS-002 and SrTiO3.structS-003 in 1,2 and 3
- Do the same for directories 1, 2 & 3 (open 3 terminals and do it in parallel):
  - *cd 1*
  - *mv SrTiO3.structS-001 1.struct*
  - *init_lapw -b -numk 10 -rkmax 6 #(batch mode)*
  - *run_lapw -fc 0.1*
  - *cp 1.scf ..*

Phonons continued

- phonopy --wien2k -f 1.scf 2.scf 3.scf
- create band.conf with editor, containing the following information:
  - *ATOM_NAME = Sr Ti O*
  - *DIM = 2 2 2*
  - *PRIMITIVE_AXIS = 1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0*
  - *BAND = 0 0 0 1/2 1/2 0 0 1/2 0 1/2 1/2 1/2 0 0 0*
  - *BAND_LABELS = G M X R G*
  - *BAND_CONNECTION = .TRUE.*
- phonopy --wien2k -c SrTiO3.struct band.conf –p
- save with: phonopy --wien2k -c SrTiO3.struct band.conf –p –s #(pdf format)
- your result should be like:

phonons are unstable because $SrTiO_3$ has distorted, tetragonal structure at low temperatures