First principles calculation of superconductivity with ABINIT

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- Introduction to electron-phonon coupling
- Eliashberg superconductivity
- ABINIT electrons and phonons
- An example
- What we don't have yet
- Conclusions?

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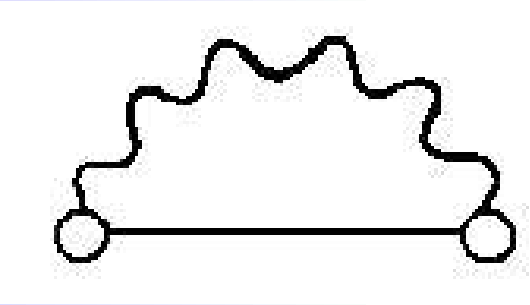
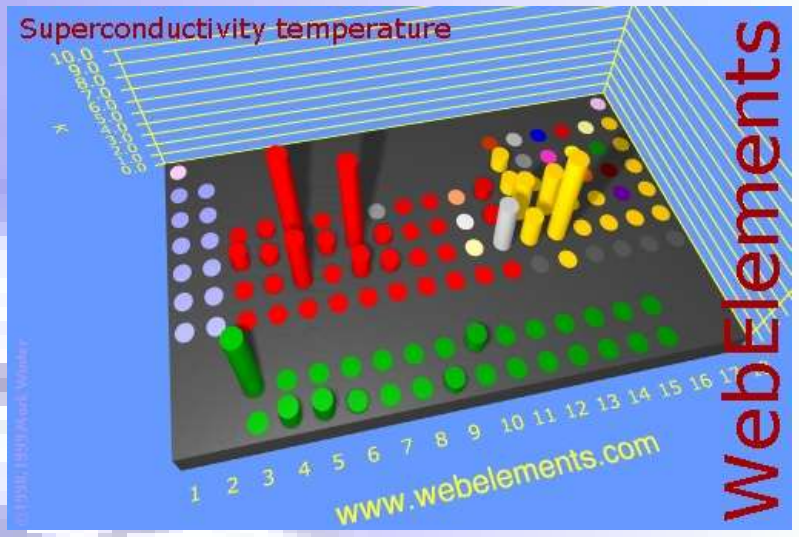
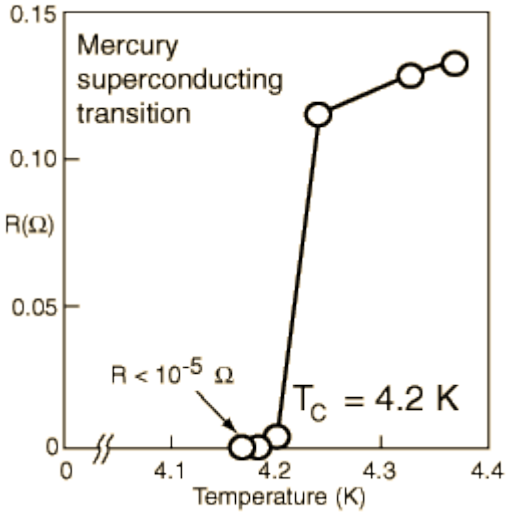
- Perfect crystal → ideal electronic states and no resistivity
- Electron-ion interaction is periodic etc...
- Renorm. electronic states (screened ions), but still ideal
- In real system, perturbations modify Hamiltonian and give finite lifetimes for eigenstates.
- External perturbations = photons, defects, impacts...

- Lowest energy perturbations = collective vibrations of nuclei → phonons. Energy packet can be localized.
- Displacement will perturb electronic density
- → Coupling between electrons and phonons
- Retardation in electronic screening of ionic movement
- And energy/frequency dependency → Kohn anomaly



- Which electronic states interact with which phonons?
- For metals, electrons at the Fermi surface
- Migdal “theorem” → only 1 phonon interaction is needed
- Actually, could be invalid, e.g. for strong correlations





- Effective interaction between electrons in presence of a phonon can be attractive → pairing +k↑ -k↓
- → superconducting instability at low T
- New "mixed" quasiparticles have no resistance.

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- Must include phonons and electrons explicitly
- Include Coulomb interaction
- Coupling Hamiltonian: $H_{ep} = \sum_{kq} \langle \boldsymbol{k+q} | \delta V | \boldsymbol{k} \rangle \boldsymbol{d_q} c^{\dagger}_{k+q} c_k$
- Perturbed (electronic) potential δV
- Displacement operator $\boldsymbol{d_q} = \sum_j \left(\frac{\hbar}{2 N M \omega_{qj}} \right) \boldsymbol{u}_{qj} (a_{qj} + a^{\dagger}_{-qj})$
- Matrix elements: $g^{qj}_{k'k} = \frac{\hbar}{\sqrt{2 N M \omega_{qj}}} \boldsymbol{u}_{qj} \langle \boldsymbol{k'} | \delta V | \boldsymbol{k} \rangle$

- Eliashberg spectral function: $\alpha^2 F(\Omega) = N_F \sum_{kk'} |g^{qj}_{k'k}|^2 \delta(\Omega - \omega_{qj})$
- Superconducting strength (or mass renormalization factor): $\lambda = 2 \int \frac{d\Omega}{\Omega} \alpha^2 F(\Omega)$
- Phonon linewidth = finite lifetime due to scattering with electrons: $\gamma_{qj} = \sum_{k \in FS} |g^{qj}_{k+qk}|^2$

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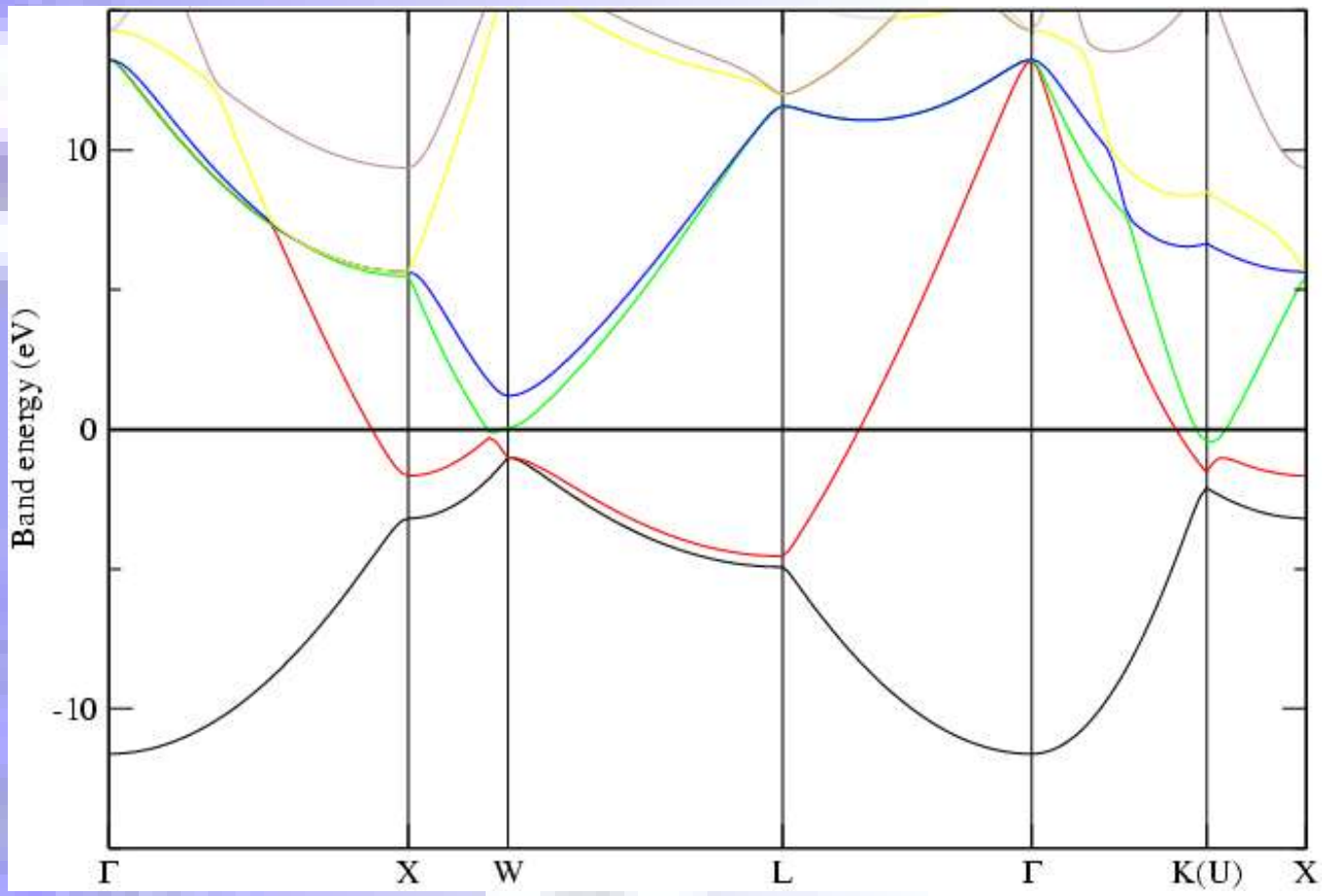
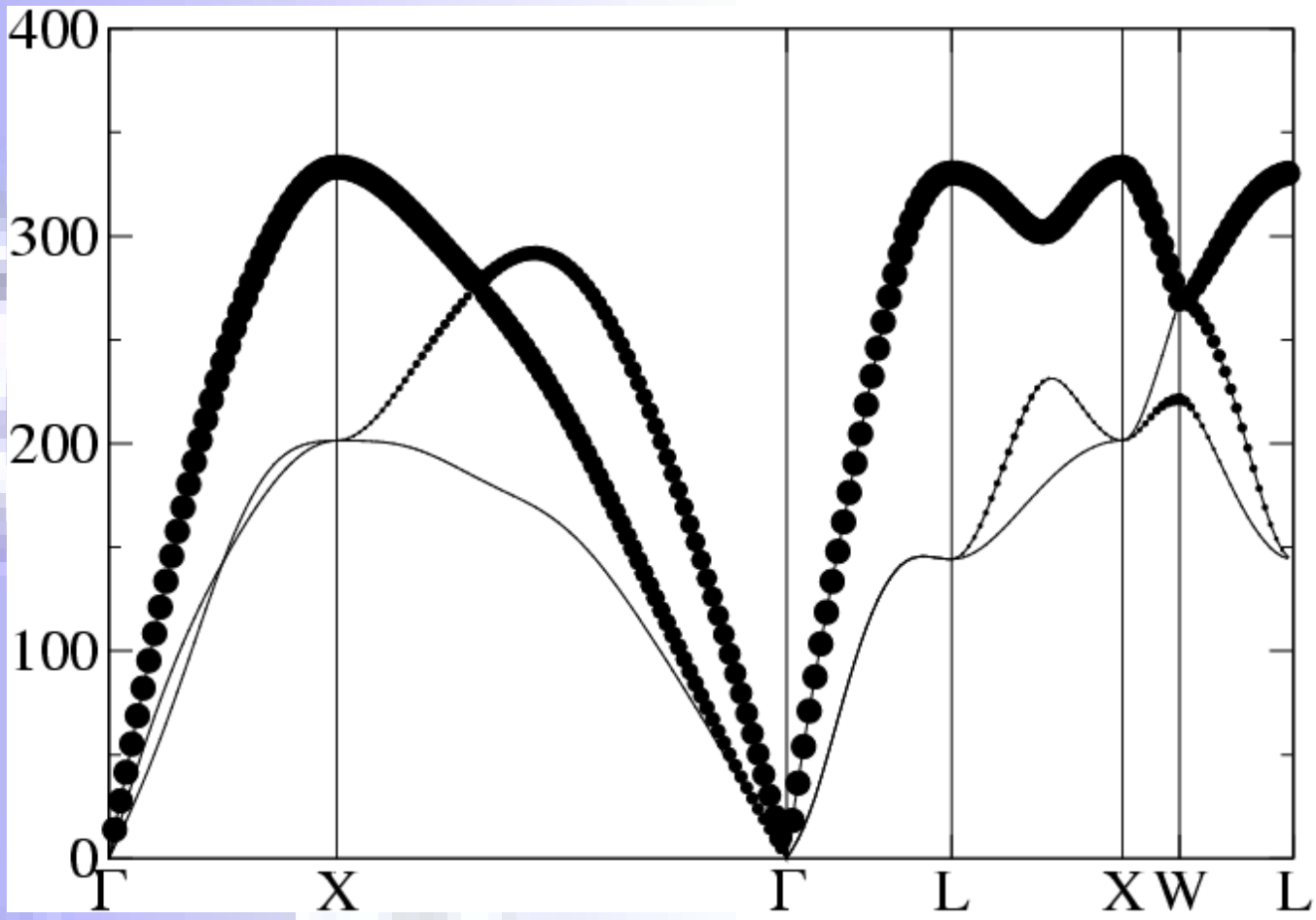


FCC Al

- BS defines Fermi Surface → need many kpoints
- Gives GS wavefunctions too

```
nshiftk 1
shiftk 0.0 0.0 0.0
ngkpt 4 4 4

tolwfr1 1.0d-14

prtden1 1

acell 3*7.5
rprim
 0.0 0.5 0.5
 0.5 0.0 0.5
 0.5 0.5 0.0
```

```
iscf 3
kptopt1 3
ecut 4.0

nband 10
occopt 7
tsmear 0.001
natom 1
typat 1
xred 0.00 0.00 0.00
nstep 800
ntypat 1
znucl 13
```



- Phonon frequencies and eigenvectors in whole BZ
- + electron-phonon interaction

```
iscf2    -3
tolwfr2  1.0d-14
getden2  1
kptopt2  3
nqpt2  1
qpt2   0.0 0.0 0.0
```

```
rfatpol3  1 1
rfdir3  1 0 0
rfphon3  1
tolvrs3   1.0e-5
getwfk3  1
getwfq3   2
kptopt3  3
nqpt3  1
qpt3   0.0 0.0 0.0
```

```
rfatpol4  1 1
rfdir4  0 1 0
rfphon4  1
tolvrs4   1.0e-5
getwfk4  1
getwfq4   2
kptopt4  3
nqpt4  1
qpt4   0.0 0.0 0.0


rfdir5  0 0 1
...
```

```
iscf6    -3
tolwfr6  1.0d-14
getden6  1
kptopt6  3
nqpt6  1
qpt6   0.5 0.0 0.0
```

```
rfatpol7  1 1
rfdir7  1 0 0
rfphon7  1
tolvrs7   1.0e-5
getwfk7  1
getwfq7   2
kptopt7  3
nqpt7  1
qpt7   0.5 0.0 0.0
```

```
rfatpol8  1 1
rfdir8  0 1 0
rfphon8  1
tolvrs8   1.0e-5
getwfk8  1
getwfq8   2
kptopt8  3
nqpt8  1
qpt8   0.5 0.0 0.0


rfdir9  0 0 1
...
```

- Phonon calculation evolves $\psi^{(1)}$ and $n^{(1)}$ to find $E^{(2)}$
- We need to calculate $\langle \boldsymbol{k}'|\delta V|\boldsymbol{k}\rangle$ and $\omega_{qj}, \boldsymbol{u}_{qj}$ (i.e. phonons)
- First order Hamiltonian (δV) is screened in phonon calculation → full convergence of $n^{(1)}$ (not bare phonons)
- Adding a new electron-phonon coupling → some double counting, but perturbation is much smaller (use in Σ_{el})

Symmetries

- Symmetry operations complete $E^{(2)}$, but phase differences preclude using them for $\langle \boldsymbol{k}'|\delta V|\boldsymbol{k}\rangle$
- $\langle \boldsymbol{k}'|\delta V_{qj}|\boldsymbol{k}\rangle\langle \boldsymbol{k}|\delta V_{qj'}|\boldsymbol{k}'\rangle$ eliminates gauge freedom
- → need all $3N_{atom}$ perturbations! But then qpoints can be completed by symmetry
- k and k'=k+q must be on FS so qpt grid must be consistent

- In ABINIT: _DDB files contain $E^{(2)}$ and _1WF files contain $\psi^{(1)}$ along with our precious $\langle \boldsymbol{k}'|\delta V|\boldsymbol{k}\rangle$
- mrgddb pastes together all $E^{(2)}$ into one file for phonons
- mrggkk extracts $\langle \boldsymbol{k}'|\delta V|\boldsymbol{k}\rangle$ and pastes them into one file
- $3N_{atom}$ perturbations must be grouped by qpoint and complete!

MRGDDB

telphon_2o.ddb.out
Total ddb for Al FCC syst
9
telphon_1o_DS3_DDB
telphon_1o_DS4_DDB
telphon_1o_DS5_DDB
telphon_1o_DS7_DDB
telphon_1o_DS8_DDB
telphon_1o_DS9_DDB
telphon_1o_DS11_DDB
telphon_1o_DS12_DDB
telphon_1o_DS13_DDB

MRGGKK

telphon_3o_GKK.bin
0
telphon_1o_DS1_WFK
9 0 0
telphon_1o_DS3_1WF1
telphon_1o_DS4_1WF2
telphon_1o_DS5_1WF3
telphon_1o_DS7_1WF1
telphon_1o_DS8_1WF2
telphon_1o_DS9_1WF3
telphon_1o_DS11_1WF1
telphon_1o_DS12_1WF2
telphon_1o_DS13_1WF3

- Integration over FS with weights from
  - Gaussian smearing (telphint = 1) with width elphsmear
  - Tetrahedron method (telphint = 0) needs input of kptrlatt
- For interpolations and tetrahedrons, include Γ and special points for k and q grids

ANADDB

```
elphflag 1

nqpath 7
qpath
 0.0 0.0 0.0
 1/2 1/2 0.0
 1   1   1
 1/2 1/2 1/2
 1/2 1/2 0.0
 1/2 3/4 1/4
 1/2 1/2 1/2

mustar 0.136
```

```
ngqpt 2 2 2
nqshft 1
q1shft 0.0 0.0 0.0

asr 2
dipdip 1
brav 1
ifcflag 1
ifcana 1
natifc 0
atifc 1 2 3
dieflag 0
eivec 1
nph11 1
qph11  0.00  0.00 0.00 1
```

ANADDB

```
elphflag 1

telphint 0
kptrlatt 4 0 0  0 4 0  0 0 4
elphsmear 0.01

nqpath 7
qpath
 ...

mustar 0.136
```

```
ngqpt 2 2 2
nqshft 1
q1shft 0.0 0.0 0.0

asr 2
dipdip 1
brav 1
ifcflag 1
ifcana 1
natifc 0
atifc 1 2 3
dieflag 0
eivec 1
nph1l 1
qph1l  0.00  0.00 0.00 1
```

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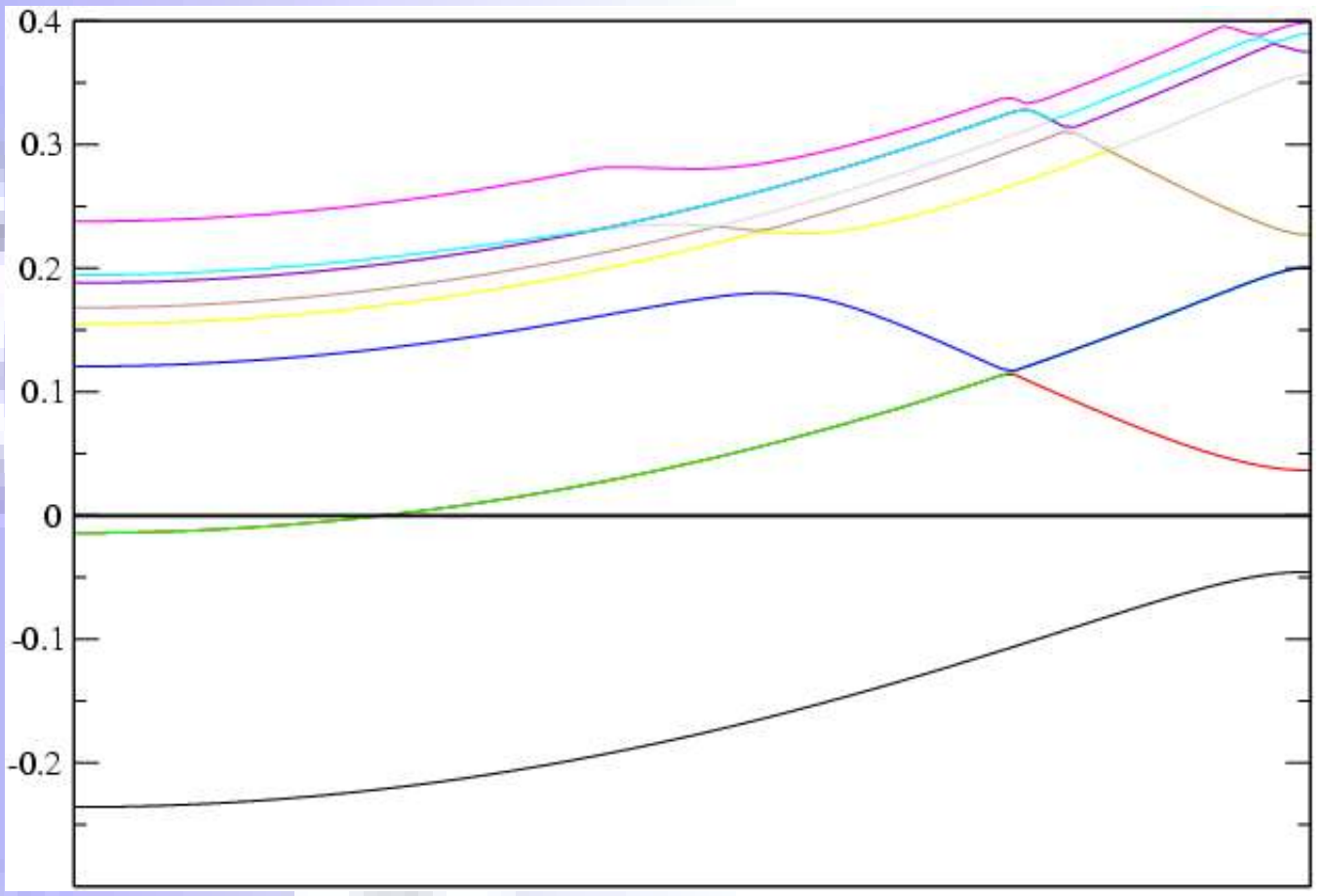
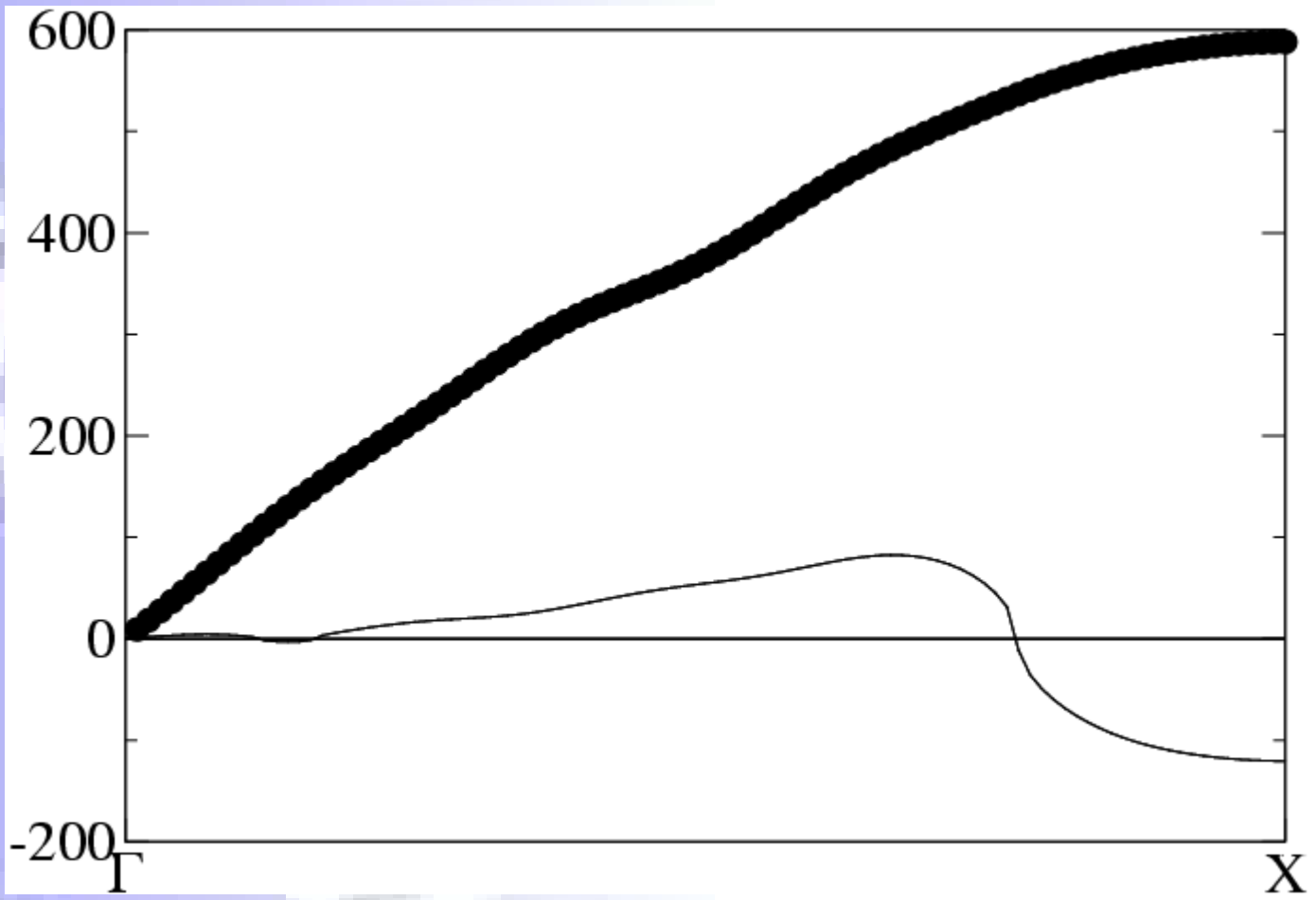
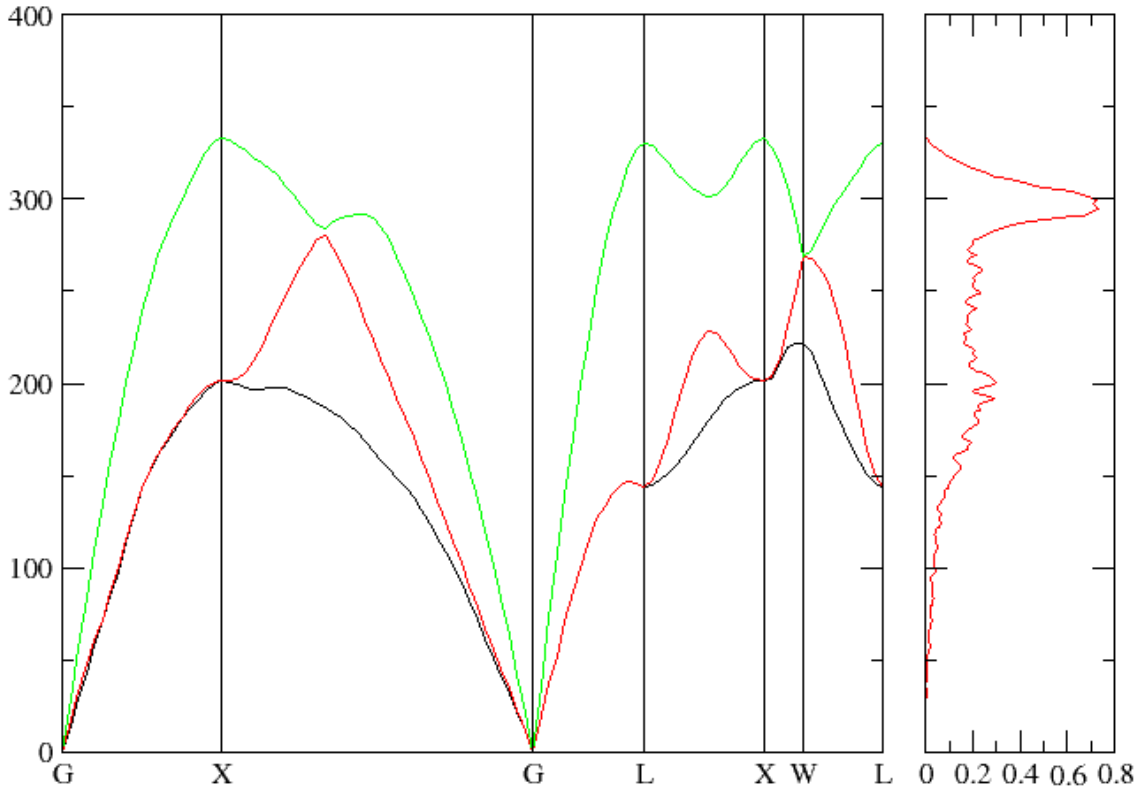


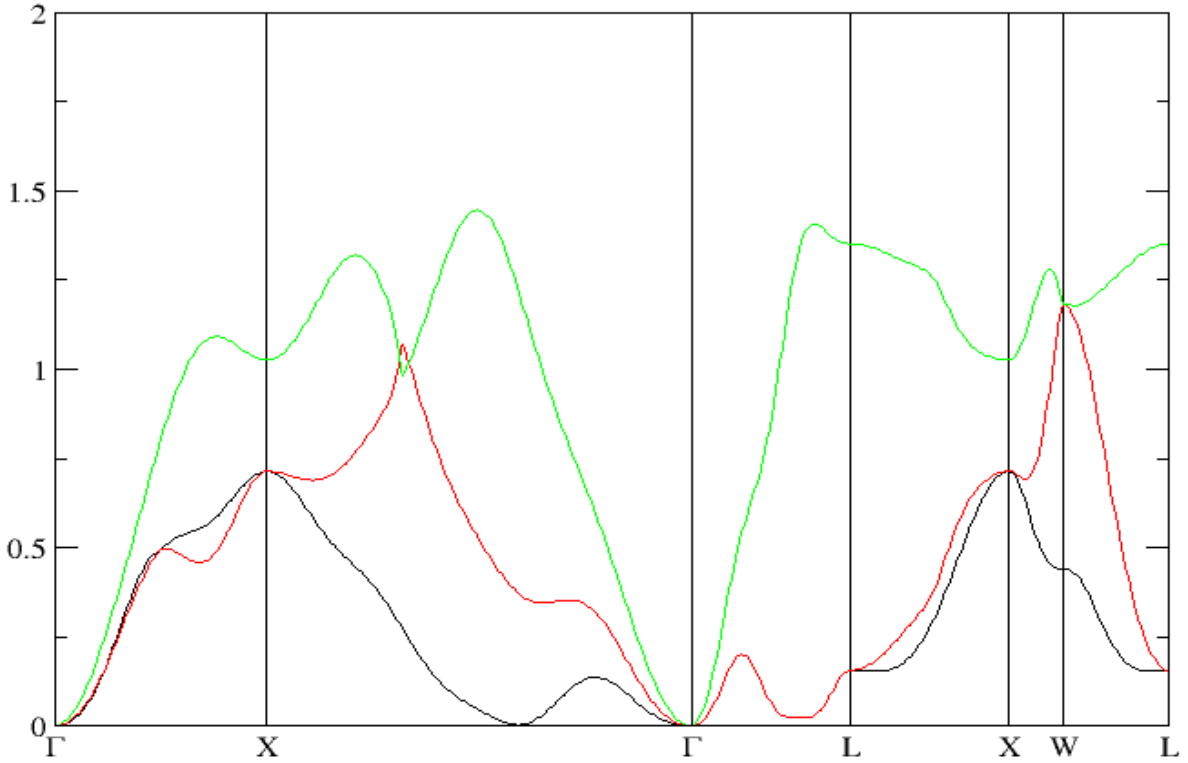
- Al monowire electronic BS
- Get _WFK and _DEN



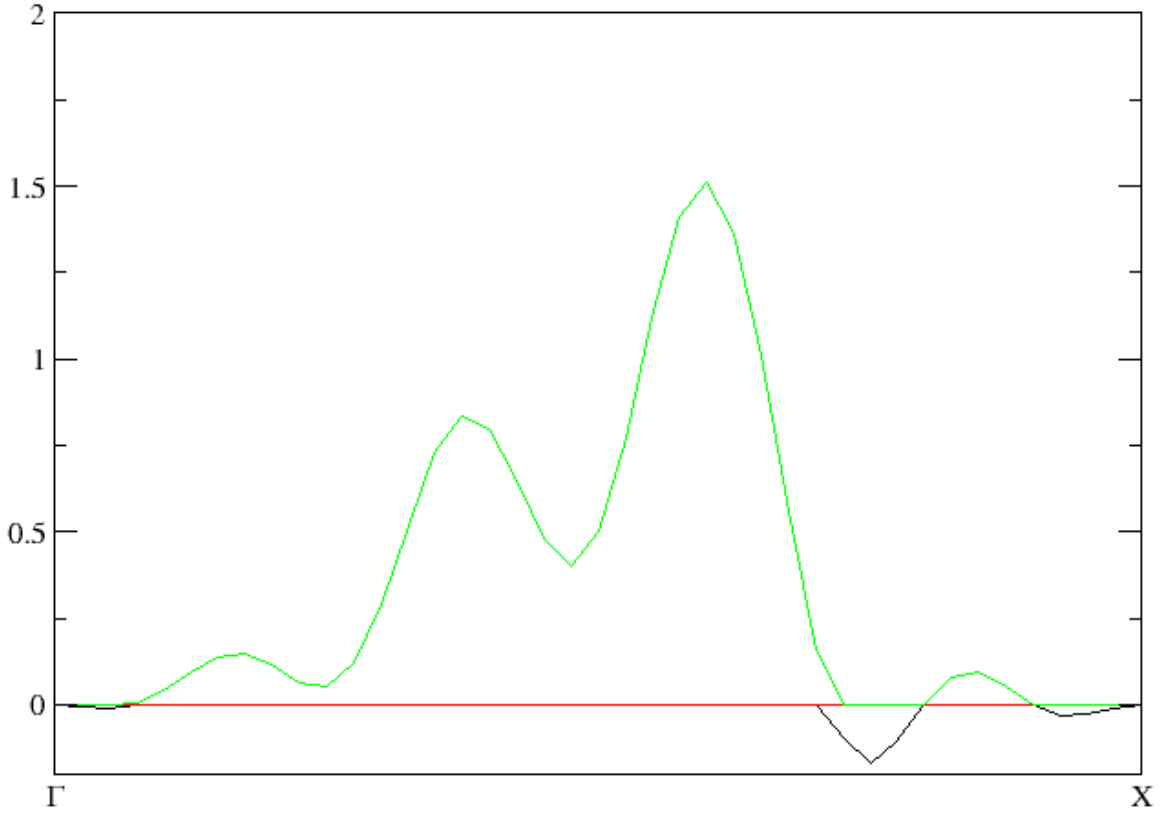
- Phonon BS: transverse modes unstable at X



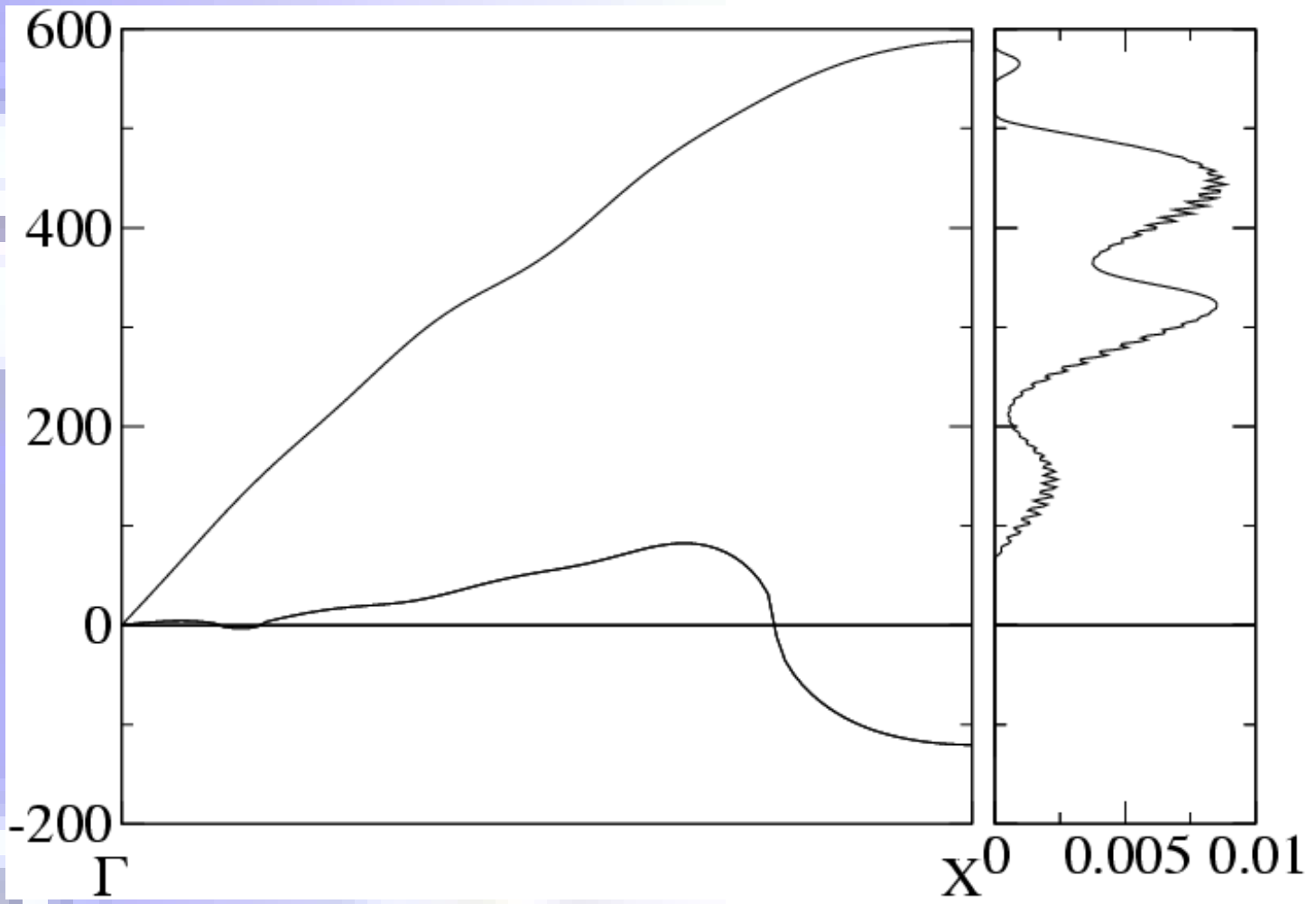
- FCC Al has strongest modes between Γ and X or Γ and L



- Phonon linewidths for FCC Al



- Wire phonon linewidths: transverse modes = no coupling



- α^2F: unstable modes have little coupling to electrons. Small overall coupling (100 times smaller than fcc)

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- Anisotropic quantities (ie. not FS averaged)
- Band resolution (not used)
- MgB2 is still not doable
- Fermi level tuning (insulators...)
- Gross Scheme
- Better Coulomb interaction

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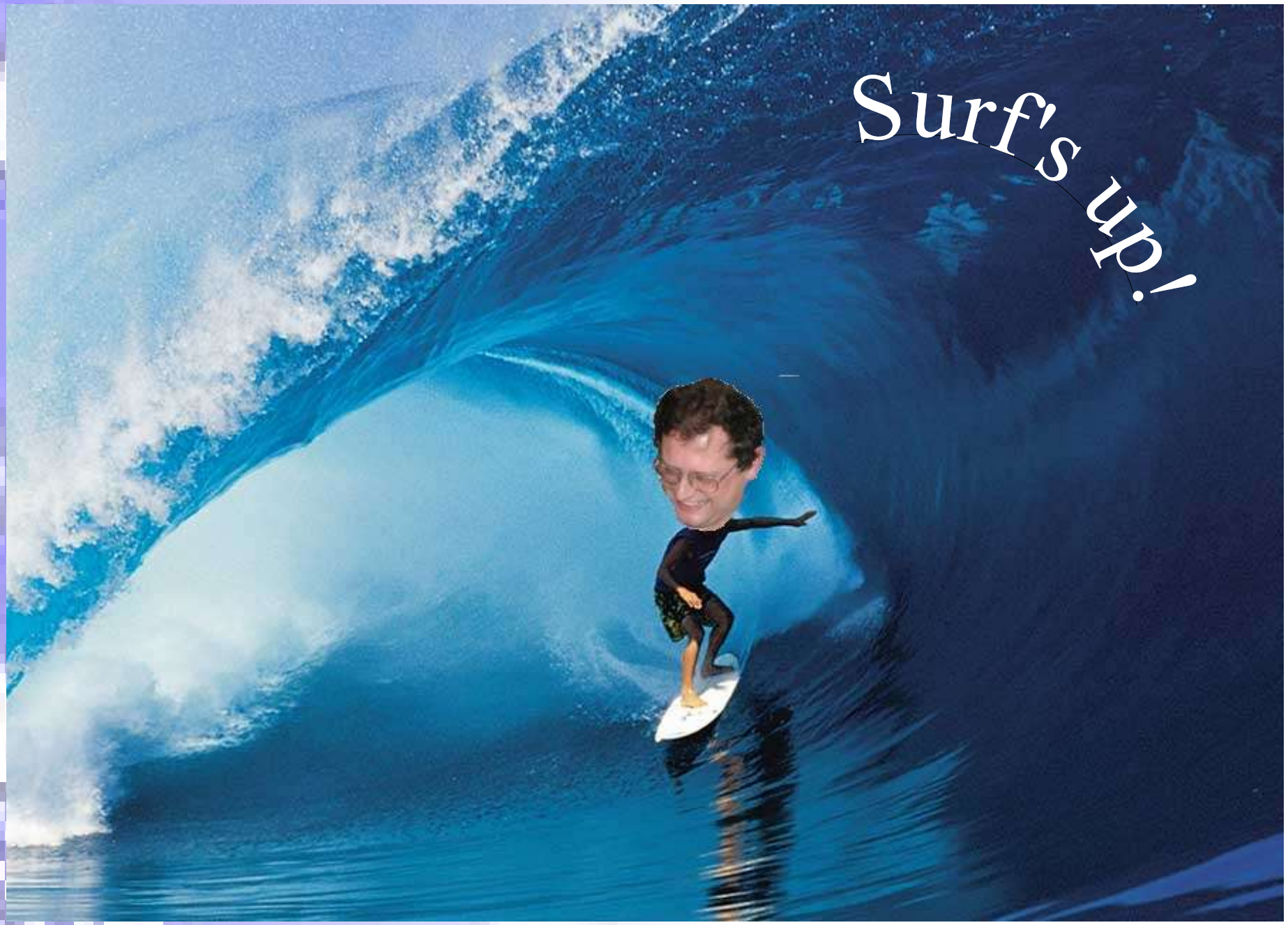
- Approaching production for small systems (low natom)
- Phonon calculation is prohibitive step (nkpt, nqpt)
- Most systems need better Coulomb or anisotropy
- Electron-phonon interaction well modeled nevertheless
- Need lots of user testing and optimization...


Surf's up!