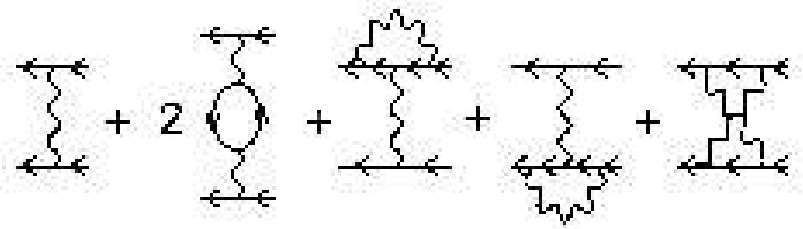
The electron-phonon interaction in ABINIT



Overview

- General introduction
- Formalism
- Implementation
  - Datastructures
  - Subroutines
- Present status

General Introduction

- El – phon interaction enters in
  - Resistivity
  - Superconductivity
  - Spectroscopies (Raman...)

- BO – approximation
- Independent quasiparticles, then coupled
  (see van Leeuwen PRB 69 115110
  and EKU Gross' group's publications
  Savrasov...)

Formalism

Allen & Mitrovic Sol Stat Phys 37

- Naïve approach

$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{e-ph}$$

- In ABINIT phonons from BO linear response
- Hence partially pre-screened, but it works and everybody else does it so why can't we?
- Lowest order (Migdal): 1 phonon scattering for 1 quasi-electron

Formalism II

- el-ph self energy

$$\Sigma_{ep} = T \int_{FS} \int_{\Omega} \frac{\alpha^2 F(k, k', \Omega)}{N(0)} \left(\frac{2\Omega}{\omega^2 + \Omega^2} \right) G$$

$$\alpha^2 F(k, k', \Omega) = N(0) \sum_j |g^j_{k,k'}|^2 \delta(\omega_{q,j} - \Omega)$$

- Eliashberg function
- gkk matrix elements

Formalism III

$$g^{j}_{k,k'} = \frac{1}{\sqrt{2 M \omega_{q,j}}} \epsilon_{q,j} \cdot \langle k | \nabla V | k' \rangle$$

- From linear response we have
  - The matrix elements
  - The phonon frequencies & eigenvectors

Formalism IV

- Mass enhancement parameter λ is 1st inv moment

$$\lambda(k,k',\omega)=\int_0^\infty d\Omega \frac{2\Omega}{\omega^2+\Omega^2}\alpha^2 F(k,k',\Omega)$$

- Phonon line widths:

$$\gamma_{q,j}=2\pi\omega_{q,j}\int_{FS}|g^{qj}_{k+q,k}|^2$$

Formalism V

- McMillan isotropic Tc formula:

$$T_c = \frac{\omega_{\log}}{1.2} \exp\left(\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right)$$

- log average frequency:

$$\omega_{\log} = \exp\left(\frac{2}{\lambda}\int_0^\infty d\Omega\, \alpha^2 F(\Omega) \frac{\ln(\Omega)}{\Omega}\right)$$

Formalism VI

- Eliashberg anisotropic equations:

$$Z(k,n) = 1 + \frac{\pi T}{|\omega_n| N(0)} \sum_{k' \in FS, n'} \lambda(k,k';n-n') s_n s_{n'}$$

$$Z(k,n)\Delta(k,n) = \pi T \sum_{k' \in FS, n'} \frac{1}{N(0)|\omega_{n'}|} [\lambda(k,k';n-n') - \mu^*] \Delta(k',n')$$

- Solve for Tc such that largest eigenvalue of kernel is 1
- Linearize equations around isotropic solution, or
- Brute force...

Implementation

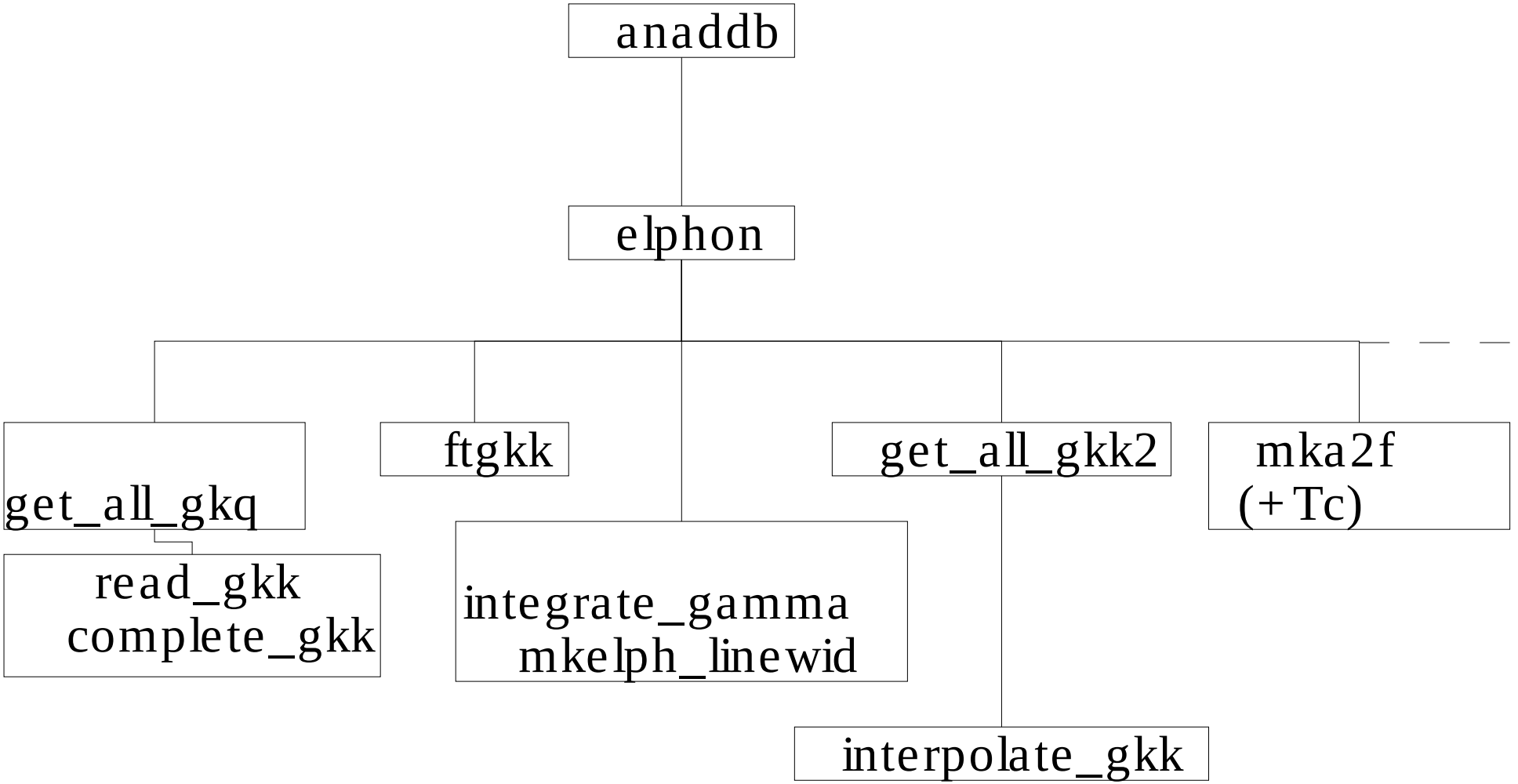
- Post-processing job in anaddb
  - Phonon runs for all modes and minimal qpoints,
  - mrggkk: Extract matrix elements which are by-product in 1WF files
  - Then 3 steps in data processing:
    - $|gkk|^2$ matrix elements in recip space
    - FT in real space
    - $|gkk|^2$ on dense kpoint grid used for respfn

Implementation II

- Characterize Fermi surface (gaussian smearing gives weighted sum over kpts)
- New elph_type datatype for $|gkk|^2$ and dims, files ...
- And, optionally, keep large matrices on disk

- Calculate linewidths
- Calculate α^2F, ω_{log}, McMillan Tc.

Implementation III



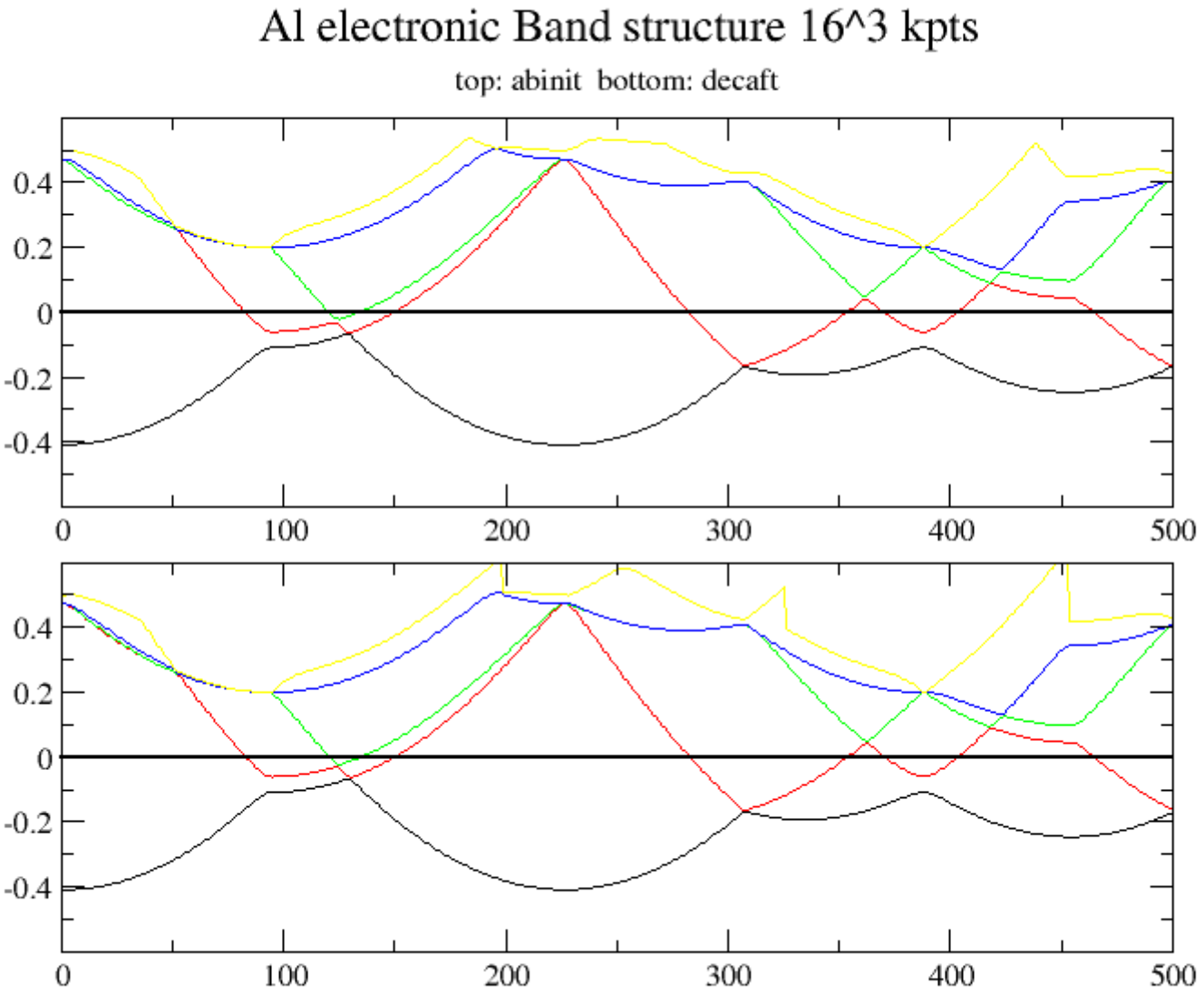
Present Status

- Test bench: FCC aluminium
- Reproduce results from DECAFT (could use PWSCF…)
- All isotropic calculations are implemented (not functional though)
- Debugging/Testing phase

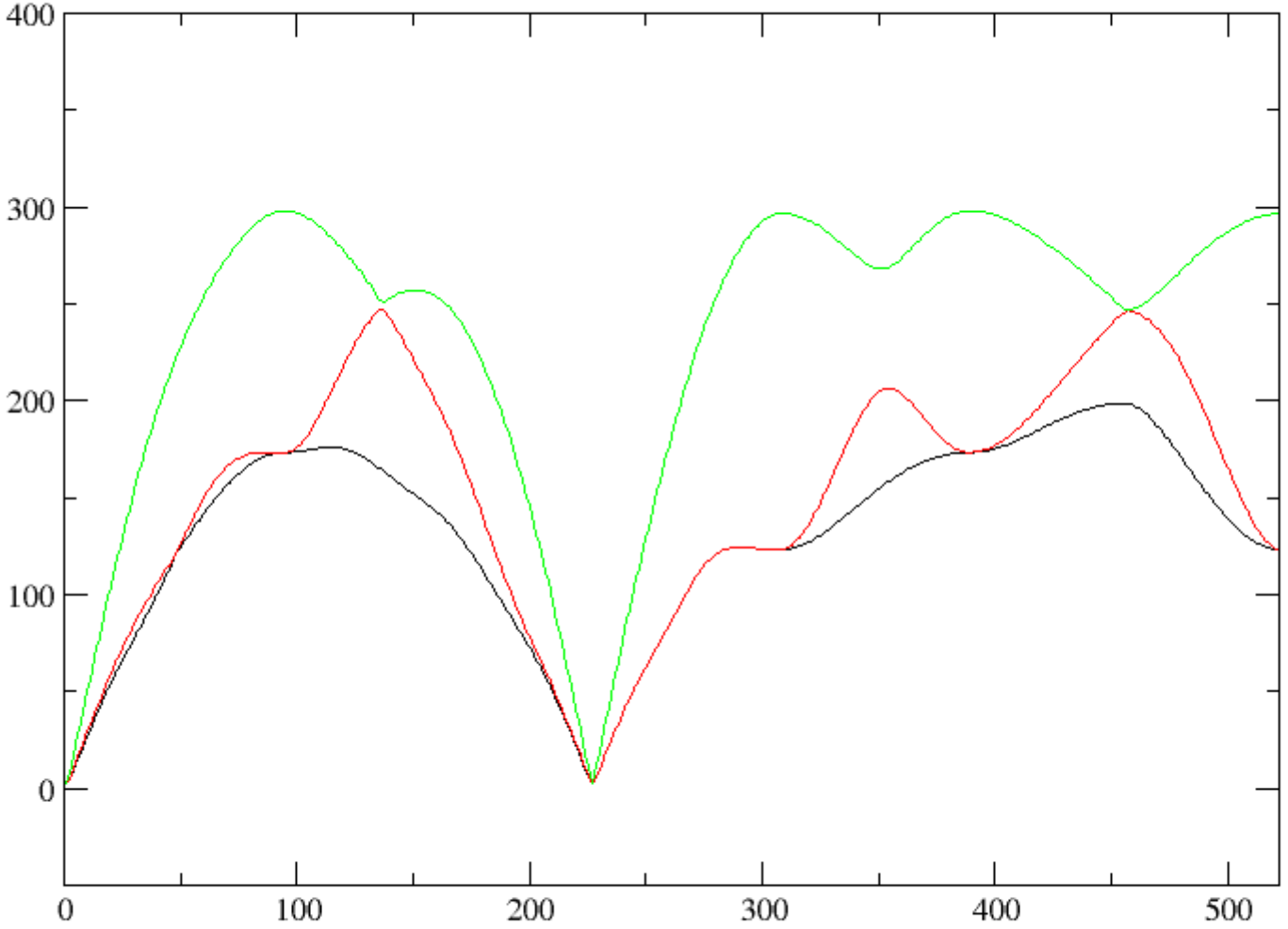
Present Status

- Symmetrization questions:
  - Phase gauge for phonon eigenvectors influences the values of phonon linewidths
  - Exploit symops to use irred qpts, perts, and kpts
- Start with no symmetries (all pert kpt qpt) and impose FCC symmetry after the fact; should this be necessary?

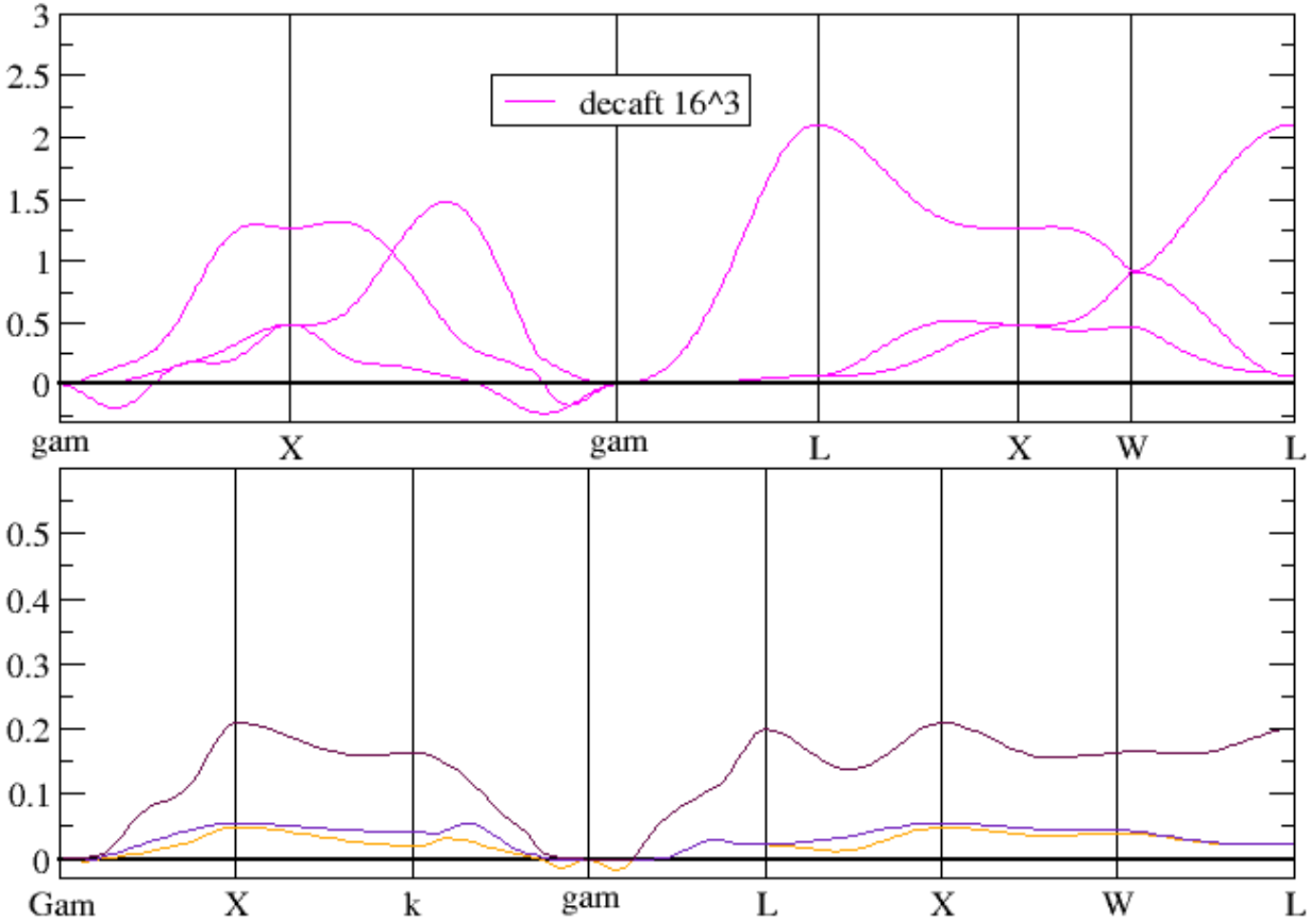
Present Status II



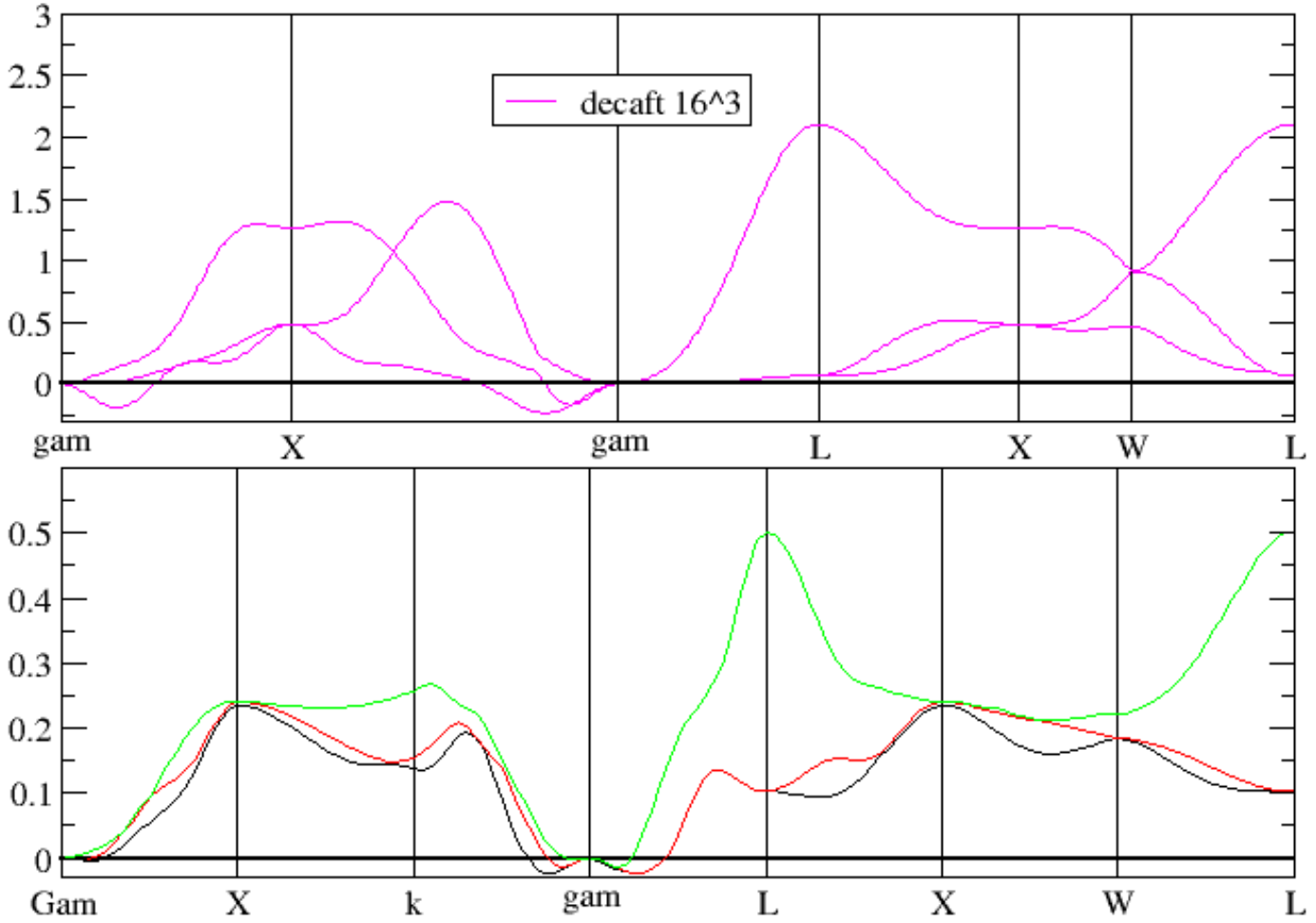
Present Status III



Present Status IV



Present Status V



Conclusions

- Should be close to our goal...
- Isotropic constants can already be of use
- Extension beyond superconductivity to other applications?
- Insulating systems... vary “Fermi energy” and sound different parts of the el-phon coupling
- Anisotropic formalism