

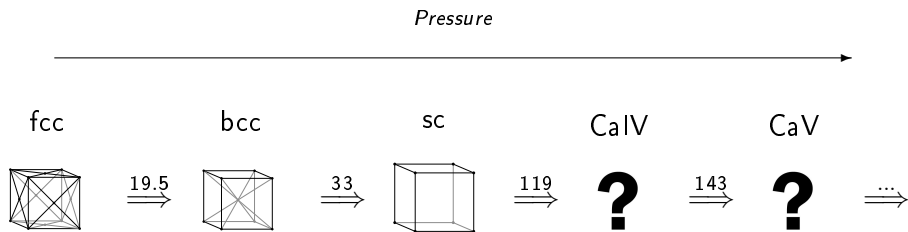
Marco Di Gennaro

*The role of the anharmonicity in the
ab-initio phase diagram of calcium*

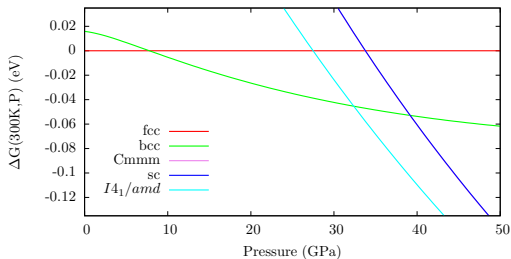
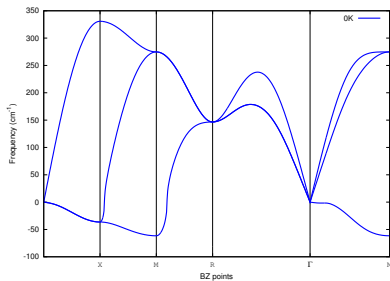
Bari Xmas Workshop December, 20th 2012

www.nanomat.ulg.ac.be

Experiment:



Theory: Sc-Ca is dynamically and thermodynamically unstable (in D.F.T.)

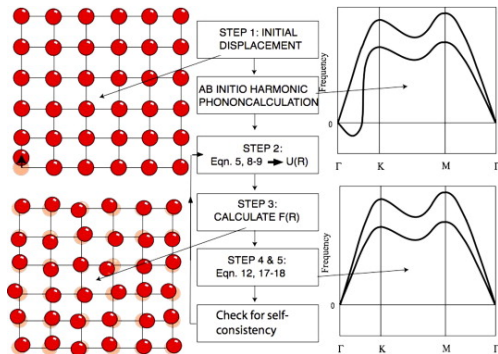


Methods: how to include temperature effects

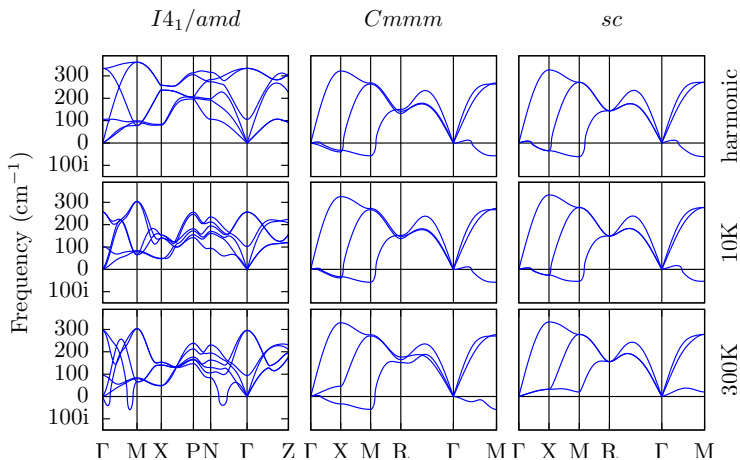
- ▶ Quasi-harmonic approximation (QHA): thermal expansion;
- ▶ Full anharmonic treatment with SCAILD:

- frozen phonon method (ph-ph interaction)
- self consistent procedure (temperature dependent)
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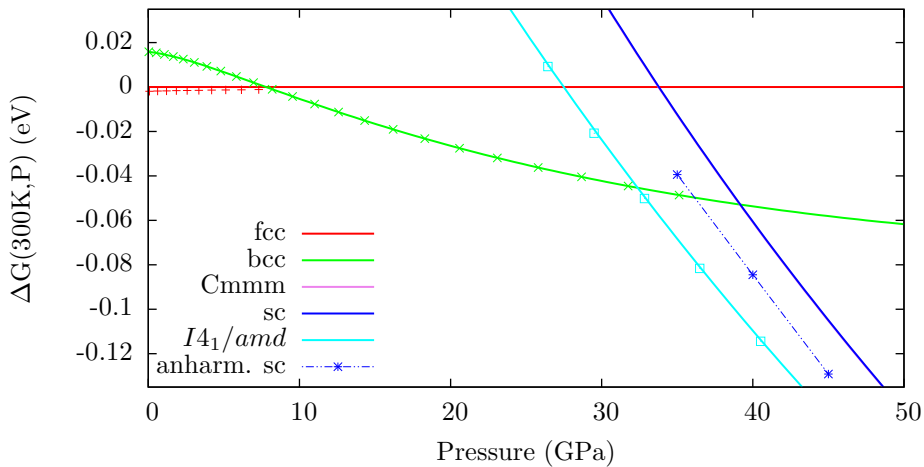
$$\mathcal{H}(\omega) \rightarrow \mathcal{H}_{harm}^{MF}(\bar{\omega})$$



Comparing phases @40GPa



Anharmonic contributions to the free energy



Conclusions

- ▶ DFPT fails in reproducing experimental phase diagram (within QHA),
- ▶ Anharmonic contribution can have different effects on different phases of the same element

- ▶ A temperature driven phase transition ($I4_1/amd \rightarrow sc$) was found
 - results submitted

- ▶ My real project (Spin-Seebeck effect):
 - longitudinal SSE, SSE on membranes, giant SSE
 - SDTT phenomena: AHE, SHE (and their inverse), ...