Current capabilities of ab initio lattice dynamics calculations

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Bandstructure methods based on density-functional theory are nowadays a standard and powerful tool for investigating electronic and structural properties of complex crystals. A modern extension, the density functional perturbation theory (DFPT), furthermore provides an efficient approach to lattice dynamical properties and related quantities within the same theoretical framework (for a recent review, see [1]). In the first part of this talk we give a brief introduction to the main concepts underlying this approach. We then present examples of current applications of DFPT to the calculation of phonon spectra for a variety of crystal structures, ranging from elemental solids to the high-temperature superconductor $Yba_2Cu_3O_7$ (see Figure 1). Results for phonons of surfaces and of one-dimensional carbon nanotubes are also discussed. These examples demonstrate the versatility and high accuracy of DFPT calculations which can thus be used to obtain reliable predictions for phonon properties of crystals for which no experimental information is available. Finally, we discuss the extension of DFPT to the calculation of the microscopic electron-phonon coupling parameters, which provides detailed information about transport and superconducting properties, and present its application to a number of superconductors with varying structural complexity.

References

[1] - S. Baroni, S. De Gironcoli, A. Dal Corso, P. Giannozzi, Rev. Mod. Phys. **73**, 515 (2001)
[2] - K.-P- Bohnen, R. Heid, M. Krauss, Europhys. Lett. **64**, 104 (2003)
[3] - L. Pintschovius, W. Reichardt, *Neutron Scattering in Layered Copper-Oxide Superconductors*, ed. A. Furrer (Kluwer Academic Press, 1998), p. 165

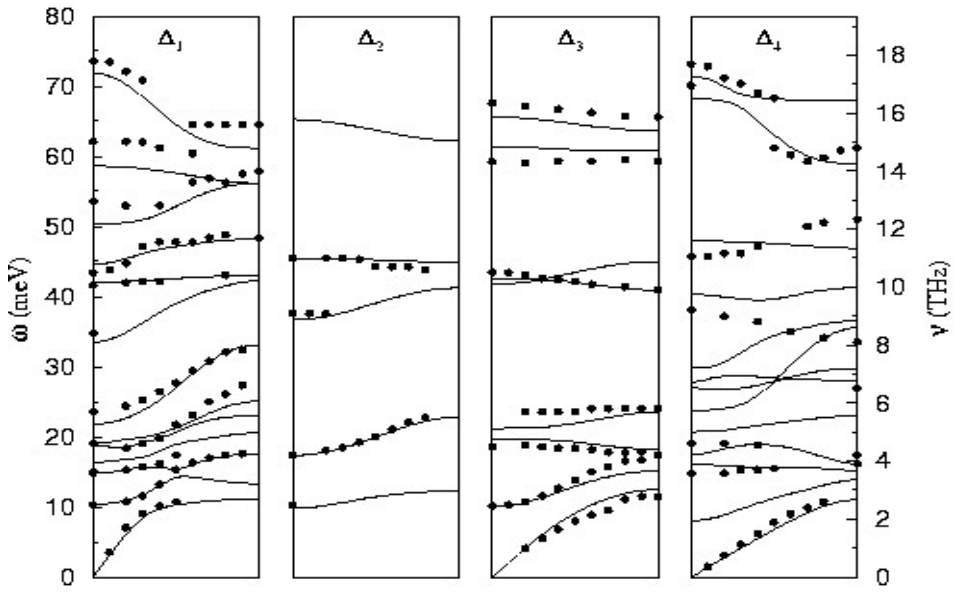

Figure 1: Theoretical phonon dispersion curves of $YBa_2Cu_3O_7$ along the [100] direction as obtained with DFPT (lines) [2]. Dots represent inelastic neutron scattering results [3].