REVIEWS OF MODERN PHYSICS, VOLUME 73, APRIL 2001

Phonons and related crystal properties from density-functional perturbation theory

Stefano Baroni, Stefano de Gironcoli, and Andrea Dal Corso Paolo Giannozzi

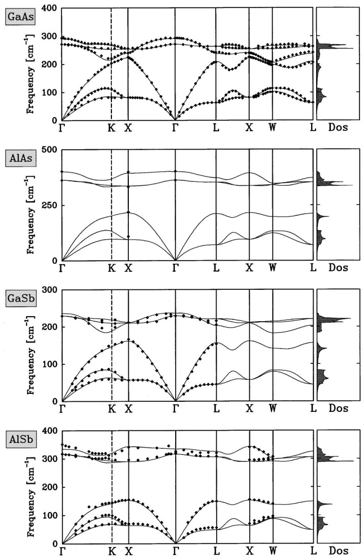

FIG. 1. Calculated phonon dispersions and densities of states for binary semiconductors GaAs, AlAs, GaSb, and AlSb: ♦, experimental data. From Giannozzi *et al.*, 1991.

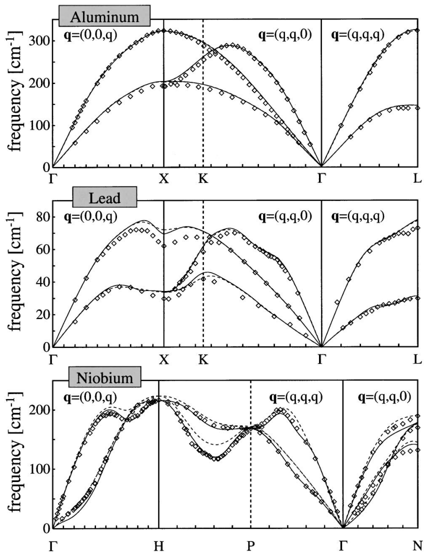

FIG. 3. Calculated phonon dispersions for fcc simple metal Al and Pb and for the bcc transition metal Nb: solid lines, 0.3 eV smearing width; dashed line 0.7 eV, smearing width; ◇, experimental data. From de Gironcoli, 1995.

$$F(q) = -\chi(q, \omega = 0),$$

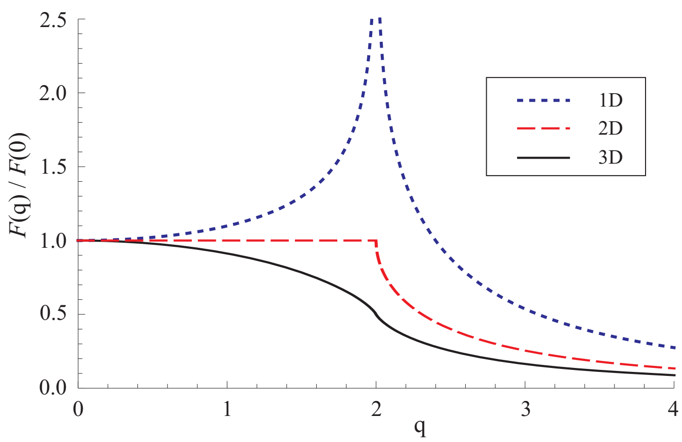

FIG. 1: (Color online) Momentum dependence of the d-dimensional static response functions, $F(q) = -\chi(q, \omega = 0)$, corresponding to zero energy transfer, $\omega = 0$. Here, momenta are expressed in rescaled units, i.e. in units of the Fermi momentum, k_F.

Kohn anomalies in 1D systems

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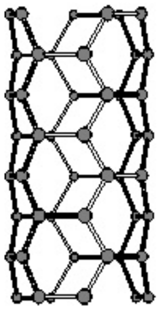
Lattice Dynamics and Electron-Phonon Interaction in (3,3) Carbon Nanotubes

K.-P. Bohnen,[1] R. Heid,[1] H. J. Liu,[2,3] and C. T. Chan[2]

(3,3)



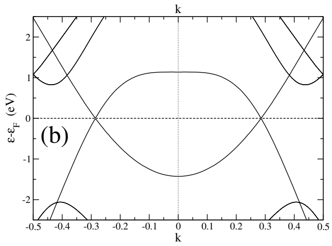


FIG. 1. Calculated band structure of the (3,3) nanotube.

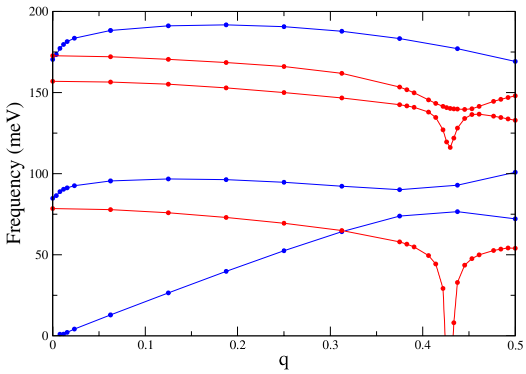


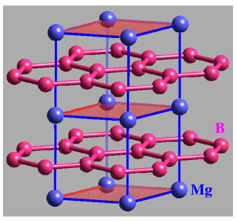
FIG. 3 (color online). Phonon dispersion curves for the two symmetry classes which are affected by electron-phonon coupling. Shown are results obtained on a fine q grid and for a small effective temperature of 137 K.

Kohn anomalies in quasi 2D systems: MgB_2

PHYSICAL REVIEW B **82**, 165111 (2010)

Adiabatic and nonadiabatic phonon dispersion in a Wannier function approach

Matteo Calandra,[1] Gianni Profeta,[2] and Francesco Mauri[1]



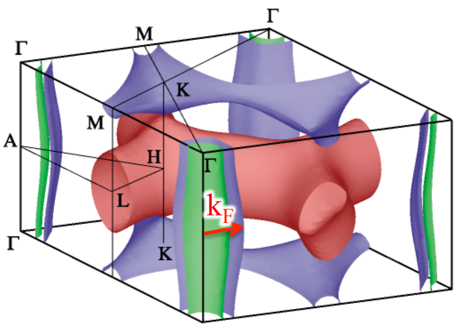


FIG. 3 (color). The Fermi surface of MgB_2. Green and blue cylinders (holelike) come from the bonding $p_{x,y}$ bands, the blue tubular network (holelike) from the bonding p_z bands, and the red (electronlike) tubular network from the antibonding p_z band. The last two surfaces touch at the K point.