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Using first-principles calculations for understanding MgB_2

JENS KORTUS, Institut de Physique et Chimie des Matériaux de Strasbourg, 23 rue du Loess, 67034 Strasbourg, France

Electronic structure methods have been the key to understand the peculiar properties of the multi-band superconductor MgB_2. After briefly reviewing the current state of our understanding of the material we will discuss some of the more recent observations on Al or C doped MgB_2.

We will demonstrate, based on first-principles band structure calculations and Eliashberg theory, that the experimentally observed decrease of the critical temperature T_c of Al and C doped MgB_2 samples can be understood mainly in terms of a band filling effect due to the electron doping by Al and C. A simple scaling of the electron-phonon coupling constant λ by the variation of the density of states (DOS) as function of electron doping is sufficient to capture qualitatively the observed behavior. Using the virtual crystal approximation to account for the electron doping we calculate the change of the DOS due to doping. The expected hardening of the E_{2g} phonon frequency at Γ is also well reproduced by our calculations using this approximation. These two contributions together, the change of DOS and phonon frequency, reproduce the observed dependence of T_c on doping concentration astonishingly well not using any free parameter to fit the data.

Further, we also explain the long standing open question of the experimental observation of a nearly constant π gap as function of doping by a compensation of the effect of band filling and interband scattering. Both effects together generate a nearly constant π gap and shift the merging point of both gaps to higher doping concentrations, resolving the discrepancy between experiment and theoretical predictions based on interband scattering only.

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