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Gap anisotropy in density functional theory of the superconducting state A. FLORIS, Freie Universität Berlin Germany, A. CONTINENZA, C. FRANCHINI, E.K.U. GROSS, N.N. LATHIOTAKIS, M. LÜDERS, M. MARQUES, S. MASSIDDA, G. PROFETA, A. SANNA — The discovery of superconductivity in MgB_2 ($T_c = 39.5$K), with the clear presence of two gaps, has renewed the interest not only in electron-phonon mediated superconductivity, but also on the problem of anisotropic superconductivity. Here we use the recently introduced density functional theory of the superconducting state, that allows calculations of material-specific properties without the use of any adjustable parameters. The method, extended to $\mathbf{k}, \mathbf{k}'$ resolved matrix elements of phonon-mediated and coulomb interactions, allows for a fully $\mathbf{k}$-resolved gap structure. Within this approach, we obtain the critical temperature and the two gaps of MgB_2 in good agreement with experiment. We will report on the existence of two different gaps also in Pb, and show that this is related to the different strength of the electron-phonon coupling associated with the two bands crossing the Fermi level. The calculated anisotropy is in good agreement with experiment. The same aproach is used for Nb3Sn, where recent experiments (Guritanu et al., Phys. Rev. B 70, 184526 (2004)) point to a possible two-gap behaviour. Our calculations show how our formalism is able to capture, in absence of any ad-hoc model, the features of multi-gap superconductors.

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