MAR07-2006-020012

Abstract for an Invited Paper
for the MAR07 Meeting of
the American Physical Society

Recent progress in applications of the superconducting density functional theory[1]

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One of the great challenges of condensed-matter theory is the prediction of material specific properties of superconductors (SC) such as the critical temperature T_c or the gap at zero temperature. Recently, based on a seminal work by Oliveira, Gross and Kohn(1), an extention of density functional theory to the superconducting state (SCDFT) was introduced and applied to elemental superconductors (2). Later work showed how the method is able to describe the properties of real materials ranging from weak to strong coupling. Unique feature of the method is the ab-initio inclusion of the Coulomb interaction which, recently combined with a fully anisotropic treatment of the electron-phonon coupling, allows for a detailed description of the most important material specific properties, including the relevance of multiple gaps, in good agreement with the available experiments.

The discovery of novel electron-phonon SC provided new challenges to the method. We will report on the most recent applications, including MgB_2, alkali metals under pressure, Ca intercalated graphite and other new and traditional SC. The subtle interplay between e-ph mediated attraction and Coulomb repulsion, normally hidden by the use of the pseudopotential μ^*, will show its material-specific importance in the resulting T_c. (1) L. N. Oliveira, E. K. U. Gross, and W. Kohn, Phys. Rev. Lett. 60, 2430 (1988) (2) Marques et al., Phys Rev. B 72, 024545 (2005); M. Lueders et al., *ibid* 024546 (2005)

[1]I acknowledge financial support by MIUR under the projects PRIN2004022024 and PON-CyberSar.