Recent progress in applications of the superconducting density functional theory\textsuperscript{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\textsuperscript{(1)}, an extension of density functional theory to the superconducting state (SCDFT) was introduced and applied to elemental superconductors \textsuperscript{(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 $\mu^*$, 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., \textit{ibid} 024546 (2005)

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