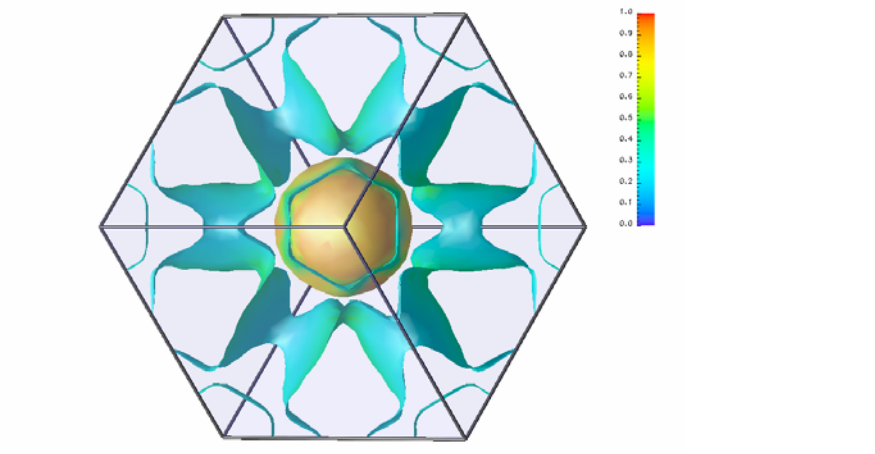
How to predict the critical temperature of superconductors: A density functional perspective

E. K. U. Gross
Institut für Theoretische Physik
Freie Universität Berlin
hardy@physik.fu-berlin.de

A novel density-functional-type approach to the description of phonon-mediated superconductivity is presented [1]. The goal of this approach is to provide a theory with predictive power, allowing the calculation of material-specific properties such as the critical temperature.To this end, the electron-phonon interaction and the electron-electron repulsion are treated on the same footing. There are no adjustable parameters such as the μ^* of Eliashberg theory. The formalism can be viewed as the superconducting generalization of the multi-component density-functional theory [2] for electrons and nuclei. Approximations of the universal xc functionals are derived on the basis of many-body perturbation theory [1,3]. Numerical results for the critical temperature and the gap will be presented for simple metals [4,5], for MgB_2 [6], and for Li, Al and K under pressure [7]. In particular, for MgB_2, the two gaps and the specific heat as function of temperature are in very good agreement with experimental data. For Li and Al under pressure, the calculations explain why these two metals behave very differently, leading to a strong enhancement of superconductivity for Li and to a clear suppression for Al with increasing pressure. For K we predict a behavior similar to Li, i.e. a strong increase of T_c with increasing pressure. Furthermore, the peculiar features of the superconducting phase of CaC_6 will be analyzed [8]. In the figure below, the gap function of CaC_6 is shown on the Fermi surface. Finally, results for hydrogen under extreme pressure will be presented. It turns out that hydrogen is a three-gap superconductor whose critical temperature increases with increasing pressure until about 100K (at 500 GPa).



[1] M. Lüders, M.A.L. Marques, N.N. Lathiotakis, A. Floris, G. Profeta, L. Fast, A.Continenza, S. Massidda and E.K.U. Gross, Phys. Rev. B **72**, 024545 (2005).
[2] T. Kreibich, E.K.U. Gross, Phys. Rev. Lett. **86**, 2984 (2001).
[3] S. Kurth, M.A.L. Marques, M. Lüders, E.K.U. Gross, Phys. Rev. Lett. **83**, 2628, (1999).
[4] M.A.L. Marques, M. Lüders, N.N. Lathiotakis, G. Profeta, A. Floris, L. Fast, A. Continenza, E.K.U. Gross, S. Massidda, Phys. Rev. B **72**, 024546 (2005).
[5] A. Floris, A. Sanna, S. Massidda and E.K.U. Gross, Phys. Rev. B **75**, 054508 (2007).
[6] A. Floris, G. Profeta, N.N. Lathiotakis, M. Lüders, M.A.L. Marques, C. Franchini, E.K.U. Gross, A. Continenza, S. Massidda, Phys. Rev. Lett. **94**, 037004 (2005).
[7] G. Profeta, C. Franchini, N.N. Lathiotakis, A. Floris, A. Sanna, M.A.L. Marques, M. Lüders, S. Massidda, E.K.U. Gross, A. Continenza, Phys. Rev. Lett. **96**, 047003 (2006).
[8] A. Sanna, G. Profeta, A. Floris, A. Marini, E.K.U. Gross, S. Massidda, Phys. Rev. B (Rapid Comm.) **75**, 020511 (2007).