chemisch
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Gegründet im Jahre 1869 von H. Hlasiwetz,
J. Loschmidt, J. Petzval und J. Stefan

EINLADUNG

zum Vortrag von

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über

How to calculate the critical temperature of superconductors?

am

Dienstag, 21. März 2006, um 17.30 Uhr

im Großen Hörsaal des Instituts für Experimentalphysik der Universität Wien
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

Abstract:
One of the great challenges of modern condensed-matter theory is to predict reliably material-specific properties of superconductors, such as the critical temperature. The traditional model of Bardeen, Cooper and Schrieffer (BCS) properly describes the universal features that all conventional superconductors have in common, but it is not able to make accurate predictions of material-specific properties. To tackle this problem, a novel density-functional approach is developed [1] which treats both the electron-phonon interaction and the electron-electron repulsion on the same footing. 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]. In this way, a true *ab initio* description is achieved which does not contain any empirical parameters. Numerical results for the critical temperature and the gap will be presented for simple metals [4], for MgB_2 [5], and for Li, Al and K under pressure. 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 [6].
[1] M. Lüders et al, Phys. Rev. B 72, 024545 (2005). [2] T. Kreibich, E.K.U. Gross, PRL 86, 2984 (2001). [3] S. Kurth, M. Marques, M. Lüders, E.K.U. Gross, PRL 83, 2628 (1999). [4] M. Marques et al, Phys. Rev. B 72, 024546 (2005). [5] A. Floris et al, PRL 94, 037004 (2005). [6] G. Profeta et al, PRL 96, (2006, in press), cond-mat/0510670.

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