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Abstract for an Invited Paper
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Density-functional theory of superconductivity¹

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A prominent challenge 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 density-functional formalism has been developed [1] which describes superconductors in thermal equilibrium in terms of three quantities: the ordinary density, the superconducting order parameter, and the nuclear N-body density. These three “densities” are determined self-consistently through a set of Kohn-Sham equations. Approximations of the universal exchange-correlation functional are derived on the basis of many-body perturbation theory. In this way, a true ab-initio description is achieved which does not contain any adjustable parameters such as the μ^* of Eliashberg theory. Numerical results for the critical temperature, the isotope effect, the gap function and the jump of the specific heat will be presented for simple metals, for MgB₂[2] and CaBeSi, and for calcium intercalated graphite (CaC₆) [3]. Furthermore, results for Li, Al, K, and H under pressure will be discussed. The calculations explain why Li and Al behave very differently, leading to a strong enhancement of superconductivity for Li and to a clear suppression for Al with increasing pressure [4]. For K we predict a behavior similar to Li, i.e. a strong increase of T_c with increasing pressure. Finally, hydrogen is found to be a three-gap superconductor whose critical temperature increases with increasing pressure until about 100K (at 500 GPa).

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