





Density Functional Theory for Superconductors: from functionals to applications

Antonio Sanna,

Max Planck Institute of Microstructure Physic, Halle, Germany

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Abstract: Density functional theory (DFT) is one of the pillars of modern material science, however it applies only to the description of the normal state. For the description of broken symmetry states (like magnetism) or temperature extensions are necessary. One of these is Density Functional Theory for Superconductors (SCDFT) where in addition to electron-electron interactions one includes also electron-phonon pairing. In this presentation I will introduce the fundamentals of SCDFT and how exchange correlation functionals have been derived via a Sham-Schlueter connection. The formalism provides an excellent framework to describe superconductivity on a fully ab-initio ground accounting for anisotropy and the effect of Coulomb interactions without empirical approximations or parameters.