A Superconductivity Density Functional Theory Based on LDA+U

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Superconducting density functional theory (SCDFT) offers an ab initio framework for evaluating superconducting transition temperatures (Tc) by treating electron-phonon coupling, screened Coulomb interactions, and spin fluctuations on a unified basis [1,2,3,4]. However, in materials with partially localized orbitals, conventional spin-fluctuation kernels may underestimate the role of local orbital correlations. In this work, we extend the spin-fluctuation part of SCDFT by incorporating a Hubbard-type local interaction inspired by LDA+U. The key ingredient is a momentum-dependent Hubbard form factor constructed from localized projector wavefunctions, allowing the local interaction to be represented consistently in the reciprocal-space basis used for the spin susceptibility.

The implementation strategy will be introduced, including the construction of the Hubbard projector form factors, their coupling to the spin-fluctuation kernel, and practical checks based on the Stoner criterion. Applications to transition-metal superconductors V and V_3Si show that the added local interaction can substantially modify the spin-fluctuation contribution and therefore the calculated Tc, even when the underlying band structure changes only weakly. This approach provides a route toward a more orbital-resolved and correlation-aware superconducting density functional theory, while also highlighting the need for careful control of effective Hubbard parameters and magnetic stability.

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