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Fe Based Superconductors from first Principles FRANK ESSENBERGER, PAWEL BUCZEK, ARTHUR ERNST, ANTONIO SANNA, LEONID SANDRATSKII, EBERHARD K.U. GROSS, Max-Planck-Institut für Mikrostrukturphysik — Density functional theory (DFT) for superconductors (SCs) is, in principle, exact and contains no adjustable parameters.[1] However, for real calculations an approximation to the pairing potential $\Delta_{\rm xc}$ is needed. Many-body perturbation theory can be used to derive approximations to $\Delta_{\rm xc}$. The perturbation series is developed in orders of the screened Coulomb and phonon interactions and truncated at the first order. Unfortunately, this approach fails to predict superconductivity in unconventional SCs, like Fe based compounds.[2] Hence, an alternative pairing mechanism has to be present in these materials, the leading contender for which is spin fluctuations.[3] We present a scheme to extend the current approximation $\Delta_{\rm xc}$ to include spin fluctuations, which involves two steps: (1) the fluctuations are calculated with time dependent DFT,[4] (2) an effective electron interaction mediated by the spin fluctuations is constructed.[5] We present results for FeSe.

[1] *Phys. Rev. Lett.*, 1988, 60, 2430
[2] *Phys. Rev. Lett.*, 2008, 101, 026403
[3] *Phys. Rev. Lett.*, 2008, 101, 057003
[4] *Phys. Rev. Lett.*, 2009, 102, 247206
[5] *Phys. Rev. B, 1985,* 32, 2156

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