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Superconductivity and Magnetism from First Principles ANDREAS LINSCHEID, ANTONIO SANNA, FRANK ESSENBERGER, E.K.U. GROSS, Max Planck Institute of Microstructure Physics — Magnetism has intriguing effects in superconductors. On the one hand static magnetic fields are known to suppress the uperconducting state while dynamic spin-fluctuations are the probable candidate to explain the pairing in the Fe-based Superconductors. Achieving an ab-initio description is important. First, because this allows to compute the critical field and whether a local coexistence of magnetic and superconducting phases exist. Second, the critical temperature of a material is among the predicted properties which allows to search yet unknown superconductors on a computer. The Density Functional Theory for Superconductors (SCDFT) has been very successful in predicting T c of phonon mediated superconductors. We include the magnetic density into SCDFT so that the electronic Kohn-Sham system now reproduces the electronic density $n(\mathbf{r})$, the order parameter of superconductivity $\chi(\mathbf{r}, \mathbf{r}')$ and the magnetic density $\mathbf{m}(\mathbf{r})$. We derive the xc-potential and discuss some first results. Furthermore, we discuss an effective electron interaction mediated by spin-flip processes based on the exact spin-susceptibility. We drive a xc-functional for SCDFT that includes this effective interaction and present some results.

Andreas Linscheid
Max Planck Institute of Microstructure Physics

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