

SELF-INTERACTION CORRECTED LOCAL SPIN DENSITY CALCULATIONS FOR SPINTRONICS MATERIALS

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Self-interaction corrected (SIC) local spin density (LSD) method is applied to study electronic structure and magnetic properties of III-V and II-VI diluted magnetic semiconductors, magnetite, and such spinel ferromagnetic insulators as NiFe_2O_4 and CoFe_2O_4 . In the diluted magnetic semiconductors we concentrate on the understanding and realization of carrier mediated ferromagnetism. The insulating charge ordered Verwey phase of magnetite is discussed in relation to the electronic structure of NiFe_2O_4 and CoFe_2O_4 , and we speculate on the implications for possible technological applications.