

DFT calculations for magnetic systems - a simple guide for non-experts

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A simple guide on first-principles calculations for non-experts will be given.

First, a brief outline of density functional theory will be provided with classification and summary of various first-principles method and name of packages. Issues with magnetism in the scope of DFT realm are listed first, and DFT approach for those properties will be reviewed - basic magnetism, magneto-crystalline anisotropy(MCA), magnetic circular dichroism (MCD), and magneto-optical Kerr effect (MOKE). Comparison with experiments and recently popular Berry phase technique will be covered as well.