Electronic Structure Theory of Materials

Prof. M. Alouani

Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504 CNRS-UdS, 23 rue du Loess, 67034 Strasbourg, France

Ab initio electronic structure methods are becoming very successful in describing and predicting the physical properties of magnetic materials due to the recent advances of high-performance computing. In the introduction chapter of this course, one learns that magnetism can not be understood within classical physics, and that its origins emerge from the symmetrization of identical particle wave functions. Equipped with the concept of symmetry, the Heisenberg Hamiltonian can be easily derived. One also learns the octahedral and tetrahedral crystal-field effects on the magnetism of transition metal ions, the super-exchange and double-exchange that lead, respectively, to antiferromagnetic and ferromagnetic coupling, and how a paramagnetic system acquires a spontaneous magnetization due to the competition between the exchange field and the electron kinetic energy. In the second part of this course, the density functional theory will be exposed. The chapter starts with the Hartree Fock approximation and the Koopmann theorem, then the Hohenberg and Kohn density functional theory (DFT) [1] will be introduced together with the concept of effective potential for solving the Kohn-Sham equations[2]. The DFT will be generalized to the case of a spin polarized fermions, and other functionals will be introduces, such as the generalized gradient approximation [3], or the so called DFT+U, where U is the Hubbard interaction among localized electrons [4]. The spin-orbit coupling and its importance in magnetism will be also discussed. In the remaining of the chapter, some applications concerning the calculation of non-colinear magnetism, spin waves, Curie temperature, magnetic anisotropy [5], and x-ray magnetic circular dichroism [6] will be discussed. After this chapter, the empirical tight-binding approximation for solving the electronic structure problem will be developed and illustrated in some simples cases, like the electronic structure of one dimensional chains or different cubic materials. The course will finish with a along chapter concerning the practical solutions of the Kohn-

Sham equations and molecular dynamics from first principles, either using the plane wave pseudopotential method [7] or all electron full-potential methods, such as the projected augmented wave (PAW) method [8] or the full-potential linear augmented plane wave (LAPW) method [9].

References:

[1] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).

[2] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).

[3] J. P. Perdew, K. Burke, and Y. Wang,Phys. Rev. B 54, 16533 (1996).

[4] V. I. Anisimov, J. Zaanen, and O. K. Andersen, Phys. Rev. B 44, 943 (1991).

[5] I. Galanakis, M. Alouani, and H. Dreyssé, Phys. Rev. B 62, 6475 (2000).

[6] V. Kanchana, G. Vaitheeswaran, M. Alouani, and A. Delin, Phys. Rev. B 75(R), 220404 (2007).

[7] Electronic Structure: Basic Theory and Proactical Methods, by R. M. Martin, Cambridge University Press, 2004.

[8] P. E. Bloechl, Phys. Rev. B **50**, 17953 (1994).

[9] Planewaves, Pseudopotentials, and the LAPW method, by David Singh and Lars Nordstrom, Springer.