TOPICS IN FUNDAMENTAL PHYSICS

[Aitor Bergara, Aritz Leonardo]

Theoretical Formalism: Introduction to Density Functional Theory (DFT) (2 ECTS)

Mode: Video lectures of the theory, assessment of challenges and problems to solve in pairs.

Introduction: What is a Kohn-Sham calculation?
Functionals: What is a functional? Functional derivatives. Euler-Lagrange equations.
One electron systems: Variational principle, trial wave-functions.
Two electron systems: Antisymmetry, Hartree-Fock and correlation.
Many electron systems: ground state and Hartree-Fock.
Density Functional Theory: Hohenberg-Kohn theorem and Thomas-Fermi.
Kohn-Sham equations: Exchange and correlations.
The Local Density Approximation: uniform electron gas.
Exchange-correlation hole: Density matrices and holes, Hooke's atom and Transferability of a hole.

Computer based simulations: Hands of DFT (2 ECTS)

Mode: Computer based practices, examples solved in pairs.

Overview of different DFT based electronic structure codes and parallel computing.

Hands on Quantum-espresso:
Solving the Kohn-Sham equation in practice: Plane waves and Pseudo-potentials
Metals versus Insulating materials: Definition of defects, surfaces and bulk.
Electronic bands, total energy and density of states calculations.
Magnetism: Non-collinear calculations and spin-orbit coupling.
Forces and structural relaxations of materials.
Phonons: Finite difference method – Phonopy.

Bibliography

R. Martin, *Electronic Structure: Basic Theory and Practical Methods,* Cambridge University Press, 2004.

C. Fiolhais, M. A.L. Marques, F. Nogueira (Eds.), *A Primer in Density Functional Theory,* Lecture Notes in Physics; Springer-Verlag Berlin Heidelberg, 2003.

D.S. Sholl and J.A. Steckel, *Density Functional Theory: A practical Introduction,* Willey, 2009.

K. Burke, *The ABC of DFT,* Department of Chemistry, University of California, Irvine, 2007.

C.A. Ullrich, *Time-Dependent Density-Functional Theory: Concepts and Applications,* Oxford University Press, 2011.

N.W. Ashcroft and D. Mermin, *Solid State Physics,* Saunders College, 1976.

Assessment: **homework** to be delivered via egela (25%)**, computer simulations (**25%), **final workshop** where each pair of students discusses an original calculation (50%).