FACOLTÀ DI SCIENZE MATEMATICHE, FISICHE E NATURALI
DIPARTIMENTO DI MATEMATICA E FISICA "NICCOLÒ TARTAGLIA"
INTERNATIONAL DOCTORAL PROGRAM IN SCIENCE

Introduction to Density Functional Theory calculations

6 hours Course

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ABSTRACT

Materials enable the technologies that power our economy and sustain our society. Accurate and reliable theoretical modelling is needed both for the understanding of fundamental processes and for the informed design of novel materials with optimal properties. For this, simulations based on a quantum mechanical description of matter have shown their unprecedented power, due to their ability to describe the fundamental electronic interactions underlying all chemistry and materials from first-principles.

The course is aimed to furnish to PhD students a basic knowledge of Density Functional Theory, the workhorse for first-principles materials modelling. The program will start from the definition of the many-electron problem in solids showing how the Hamiltonian can be re-written in term of electronic density. This preliminary step will serve to introduce the Hohenberg-Kohn theorems and the Khon-Sham equations that are the core of DFT. Finally, some theoretical and computational aspects, such as the self-consistent approach, the choice of the density functional and basis set, the pseudopotential description of core electrons etc. will be presented. A practical hands-on session, based on one of the most widely used DFT codes (QuantumEspresso), will conclude the course with some examples of calculation of structural and electronic properties of solid-state systems.

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PhD Course

14th June 2023, 10:00-13:00 - Aula 24
Università Cattolica del Sacro Cuore
via Garzetta 48, Brescia

15th June 2023, 9:30-13:00 Laboratorio di calcolo LCM
Dipartimento di Fisica, Università degli Studi di Milano
Via Giovanni Celoria 16, Milano

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