Scuola di Dottorato in Fisica
Dipartimento di Fisica Enrico Fermi – Università di Pisa

Corso Avanzato di Struttura della Materia – a.a. 2013/14

From Mon, March 10, to Fri, March 14, 2014 – 15.00-17.00 – room 230 building C
(5 seminars)

Introduction to modeling and simulations

Francesco Puosi
Univ. Grenoble 1/CNRS, LIPhy UMR 5588, Grenoble, F-38041, France
(francesco.puosi@ujf-grenoble.fr)

This short course provides an introduction to modeling and simulations at atomistic and molecular level. Simulations provide a very powerful way of solving many-body problems in Physics, enabling one to go directly from a microscopic Hamiltonian to macroscopic properties measured in experiments, essentially without approximation. In recent years, the advance of computational power has lead to a rapid development of simulations, both in applications and methodology. The goal of this seminars is to provide you the relevant theoretical and numerical tools that are necessary to build models of physical phenomena and to simulate their behavior using computers. Molecular Dynamics (MD) and Monte Carlo (MC) methods will be discussed in detail. Emphasis will be on the connections between the simulation results and real properties of materials (structural or thermodynamic quantities), as well as numerical algorithms.