

Scuola Superiore di Catania

**Classe delle Scienze Sperimentali
Corso specialistico
ambito disciplinare: Scienze e Tecnologie**

“Introduction to computational materials physics”

a.a. 2014-2015

Module 1: Atomistic simulations of materials

- a. Introduction to molecular dynamics simulations: theoretical foundation and numerical implementation
- b. Structure evolution of complex materials under processing
- c. Thermal transport in nanomaterials
- d. Nanocomposite materials for biomedical applications

Module 2: Optoelectronic properties of materials

- a. Introduction to electronic structure calculations: theoretical foundation and numerical implementation
- b. Quantum confinement phenomena in nanoscale systems
- c. Nanostructure vs. optoelectronic properties
- d. Radiation-matter interaction: photoconversion

Module 3: Mechanical properties of materials

- a. Introduction to materials mechanics: theoretical foundation and numerical implementation
- b. Elastic behavior of nanostructured materials
- c. Elastic behavior of 2D atomic sheet: the case of graphene.