INSA INSTITUT NATIONAL DES SCIENCES APPLIQUÉES LYON

Nanotechnology

Computer modelling of nanoscale systems

IDENTIFICATION

CODE : M2-NANO-NANO-S3-8
ECTS : 3.0

HOURS

Lectures :	16.0 h
Seminars :	7.0 h
Laboratory :	7.0 h
Project :	0.0 h
Teacher-student contact :	30.0 h
Personal work :	15.0 h
Total :	45.0 h

ASSESSMENT METHOD

Final written exam

TEACHING AIDS

TEACHING LANGUAGE

English

CONTACT

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AIMS

This course introduces the principles underlying common methods of numerical simulations used in the nanosciences, going from the atomistic scale to the continuum. It discusses the appropriateness of various methods according to the scale and the level of modeling, to understand the principles of the models and algorithms used in standard codes.

CONTENT

Part 1:
¿ Choice of models and methods
¿ Overview of problems and scales
¿ Atomistic models (with and without electrons)
¿ Classical molecular dynamics: from statistical mechanics to the algorithms
Part 2:
¿ Finite element methods
¿ Interpolation functions for the estimating displacements
¿ Construction of the elementary operators after discretization
¿ Governing principles and variational formulation
¿ Couples models (molecular

BIBLIOGRAPHY

Daan Frenkel, Berend Smit, "Understanding molecular simulation: from algorithms to applications", Academic press, San Diego, second edition, 2002

PRE-REQUISITE

Nanomechanics (M1)

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