Politecnico di Milano

Dottorati di Ricerca in Chimica Industriale e Ingegneria Chimica, Ingegneria dei Materiali e Bioingegneria

Multidisciplinary course offered by the Scuola di Dottorato di Ricerca

Simulation of molecular systems for chemistry, materials and biology

5 July – 9 July 2021

Polo di Lecco, Politecnico di Milano
www.polo-lecco.polimi.it

For information please contact:
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Monday July 5

9.00-9:15: ***Welcome***
9.15-10.45: ***Antonino Famulari***
Break
11.15-12.45: ***Matteo Tommasini***
Lunch
14.00-17.00: *computer practicals on QM methods (1)*
Break
17.30-18:15: Seminar 1

Tuesday July 6

9.30-10.45: ***Alberto Milani***
Break
11.15-12.45: ***Carlo Cavallotti***
Lunch
14.00-17.00: *computer practicals on MD methods (2)*
Break
17.30-18:15: Seminar 2

Wednesday July 7

9.30-10.45: ***Fabio Ganazzoli/Giuseppina Raffaini (lecture 2)***
Break
11.15-12.45: ***Matteo Maestri***
Lunch
14.00-17.30: *computer practicals on MD methods (2)*
Break
17.30-18:15: Seminar 3

Thursday July 8

9.30-10.45: ***Mosè Casalagno***
Break
11.15-12.45: ***Alfonso Gautieri***
Lunch
14.00-17.00: *computer practicals on QM methods (2)*
Break
17.30-18:15: Seminar 4
20:00-: Social Dinner

Friday July 9

9.15-12.45: ***Spare time for self study***
Break
14.00-17.00: ***Exam (Journal Club)***
Concluding remarks and farewell

Formative goals

Molecular simulation is a powerful and widely used method in materials science and engineering, biophysics, chemistry, chemical engineering, drug design and many other areas. The aim of the course is to provide a critical understanding of these methods and a practical introduction to their use.

Accommodation:

Residenza A. Loos di Lecco
Via Antonio Ghislanzoni, 24 - Lecco
Meals and the travelling expenses are not included.

Course venue

Politecnico di Milano - Polo Territoriale di Lecco
Via G. Previati 1/c - 23900 Lecco
Room B 2.2 (morning lectures) – to be confirmed
Room B 2.4 (afternoon practicals) – to be confirmed

The final exam will consist in a critical analysis of a literature paper chosen among a proposed selection (journal club).

LECTURES

Mosè Casalegno, Politecnico di Milano

Molecular Dynamics.

Aims of MD simulations. Algorithms for integration of MD equations. Constraints in simulations. Periodic boundary conditions. Neighbour lists. Treatment of long-range interactions. MD in various ensembles: thermostats and barostats. Observables from MD simulations: correlation functions.

Carlo Cavallotti, Politecnico di Milano

QC methods for the study of chemical kinetics

Conventional and variational transition state theory (TST); quantum chemical determination of TST parameters in the rigid rotor harmonic oscillator (RRHO) approximation; multi well reactions; beyond the RRHO approximation: hindered rotors and anharmonicities; RRKM/Master equation theory and its numerical solution.

Antonino Famulari, Politecnico di Milano

Quantum chemistry 1

Introduction of Born-Oppenheimer and the clamped nuclei Hamiltonian. The potential energy surface and its characterization: minimization and transition state search. Electronic wavefunctions and the independent particle model: spin, antisymmetry, Slater determinants. The Hartree-Fock method and atomic basis sets (LCAO). Ab initio and semiempirical methods.

Fabio Ganazzoli and Giuseppina Raffaini, Politecnico di Milano

Atomistic force fields and introduction to molecular dynamics

Introduction to molecular simulation and force fields. Intra- and inter-molecular potential energy: force fields for atomistic molecular models. Bond stretching, bending, torsional potentials, etc. Harmonic and anharmonic intramolecular potentials, coupling terms. Inter-molecular potential energy: Coulombic and Lennard-Jones potentials. Force fields parametrization. An example of application.

Alfonso Gautieri, Politecnico di Milano

Modelling and Engineering of Biomolecules

Structure and molecular dynamics simulations of biomolecules. Advanced sampling: binding and free energy calculations, metadynamics, accelerated molecular dynamics, replica exchange molecular dynamics, coarse-grained modelling. Biomolecular engineering: protein folding, rational protein engineering, de novo protein structure prediction and design.

Matteo Maestri, Politecnico di Milano

Ab initio MD simulations.

Motivation for ab initio MD. Density functional theory for periodic systems: Bloch theorem, plane-wave basis sets. Integration methods: the Car-Parrinello algorithm. Application examples: materials, surfaces and catalysis.

Alberto Milani, Politecnico di Milano

Molecular Spectroscopy

Introduction to molecular spectroscopies and observables. Quantum chemical calculation of spectroscopic properties: in-depth discussion of IR and Raman vibrational spectra, elements of molecular excited states and UV-VIS spectra.

Matteo Tommasini, Politecnico di Milano

Quantum chemistry 2

Introduction to electron correlation: configuration interaction and excited states. The electron density and its interpretation: dipole moments, molecular electrostatic potential, atomic charges. Introduction to Density Functional Theory: Hohenberg & Kohn theorem and Kohn-Sham method. Extensions to open shell systems. Chemical reactions and the bond-breaking problem.