Chimica Computazionale

Introduction

Emanuele Coccia

UNIVERSITÀ DEGLI STUDI DI TRIESTE

DSCF Dipartimento di Scienze Chimiche e Farmaceutiche

PhotoInduced Quantum Dynamics (PIQD) Group

PIQD

Practical info

- ecoccia@units.it
- C11 building, fourth floor, room 453/454
- Just send an email to get an appointment
- Register on Moodle

Programme

- **Introduction to computational chemistry**
  - Definition of computational chemistry
  - Math overview

Programme

- **Introduction to computational chemistry**
  - Definition of computational chemistry
  - Math overview
- **Fundamentals of quantum chemistry**
  - Fundamentals of quantum mechanics (QM)
  - Born-Oppheneimer approximation
  - Hartree-Fock method
  - Basis sets
  - Configuration Interaction
  - Density functional theory

Programme

- **Introduction to computational chemistry**
  - Definition of computational chemistry
  - Math overview
- **Fundamentals of quantum chemistry**
  - Fundamentals of quantum mechanics (QM)
  - Born-Oppheneimer approximation
  - Hartree-Fock method
  - Basis sets
  - Configuration Interaction
  - Density functional theory
- **Molecular mechanics and dynamics**
  - Molecular mechanics (MM)
  - Molecular dynamics
  - Monte Carlo method
  - Statistical thermodynamics

Programme

- **Introduction to computational chemistry**
  - Definition of computational chemistry
  - Math overview
- **Fundamentals of quantum chemistry**
  - Fundamentals of quantum mechanics (QM)
  - Born-Oppheneimer approximation
  - Hartree-Fock method
  - Basis sets
  - Configuration Interaction
  - Density functional theory
- **Molecular mechanics and dynamics**
  - Molecular mechanics (MM)
  - Molecular dynamics
  - Monte Carlo method
  - Statistical thermodynamics
- **Hybrid multiscale schemes**
  - QM/MM methods
  - Polarizable continuum models

Programme

- **Introduction to computational chemistry**
  - Definition of computational chemistry
  - Math overview
- **Fundamentals of quantum chemistry**
  - Fundamentals of quantum mechanics (QM)
  - Born-Oppheneimer approximation
  - Hartree-Fock method
  - Basis sets
  - Configuration Interaction
  - Density functional theory
- **Molecular mechanics and dynamics**
  - Molecular mechanics (MM)
  - Molecular dynamics
  - Monte Carlo method
  - Statistical thermodynamics
- **Hybrid multiscale schemes**
  - QM/MM methods
  - Polarizable continuum models
- **Geometry optimization and reaction profile**
  - Characterizing a potential energy surface
  - Minimum search
  - Transition-state search

Programme

- **Introduction to computational chemistry**
  - Definition of computational chemistry
  - Math overview
- **Fundamentals of quantum chemistry**
  - Fundamentals of quantum mechanics (QM)
  - Born-Oppheneimer approximation
  - Hartree-Fock method
  - Basis sets
  - Configuration Interaction
  - Density functional theory
- **Molecular mechanics and dynamics**
  - Molecular mechanics (MM)
  - Molecular dynamics
  - Monte Carlo method
  - Statistical thermodynamics
- **Hybrid multiscale schemes**
  - QM/MM methods
  - Polarizable continuum models
- **Geometry optimization and reaction profile**
  - Characterizing a potential energy surface
  - Minimum search
  - Transition-state search
- **Computational exercises**

Programme

- **Introduction to computational chemistry**
  - Definition of computational chemistry
  - Math overview
- **Fundamentals of quantum chemistry**
  - Fundamentals of quantum mechanics (QM)
  - Born-Oppheneimer approximation
  - Hartree-Fock method
  - Basis sets
  - Configuration Interaction
  - Density functional theory
- **Molecular mechanics and dynamics**
  - Molecular mechanics (MM)
  - Molecular dynamics
  - Monte Carlo method
  - Statistical thermodynamics
- **Hybrid multiscale schemes**
  - QM/MM methods
  - Polarizable continuum models
- **Geometry optimization and reaction profile**
  - Characterizing a potential energy surface
  - Minimum search
  - Transition-state search
- **Computational exercises**
- **Hints on machine learning**

Where studying

- Slides
- F. Jensen, *Introduction to Computational Chemistry*. UK: John Wiley & Sons
- C. J. Cramer, *Essentials of Computational Chemistry*. UK: John Wiley & Sons
- J. Harvey, *Computational Chemistry*. Oxford University Press
- Further reading: D. Frenkel and B. Smit, *Understanding Molecular Simulation: from algorithms to applications*. Academic Press

Exam

- Oral exam: (at least) three questions
- Exam done in a lecture room:
  - Two rounds in winter session
  - Two rounds in summer session
  - Two rounds in September