Chimica Computazionale

Introduction

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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

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  - Hartree-Fock method
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  - Density functional theory
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- **Computational exercises**

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