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Exercise Session 1 IESM Fall 2024-2025

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Introduction to Electronic Structure Methods

Welcome to the IESM course!

- Lecturer: Prof. Ursula Röthlisberger
- TAs:
 - Salomé Guilbert
 - Qihao Zhang
 - Thibault Kläy
 - Evan Vasey
 - Different PostDocs from LCBC lab



Introduction to Electronic Structure Methods

- Mondays from 8:15 to 10:00 and Tuesdays from 10:15 to 12:00
- Course schedule for the semester available on Moodle and the exercise webpage



Exercise sessions

• Moodle page



Introduction to electronic structure methods

Dashboard > Courses > Chimie, Génie Chimique (CGC) > CGC - Bachelor > CH-353



Exercise sessions

• Exercise website: https://lcbc-epfl.github.io/iesm-public/

Introduction to Electronic Structure Methods Q Search this book...









Introduction to Electronic Structure Methods

This book contains the script and exercises for the course CHE-351

Introduction to Electronic Structure Methods (IESM) given at EPFL.



Exercise structure

Introduction

- Learning goals
- Chapter in script
- Resources





Exercise structure

Theory section

- Relevant theory for the exercise
- Theoretical exercises

Practical exercises

- "Coding" exercises
- Interpretation of results



Exercise evaluation

Examples:

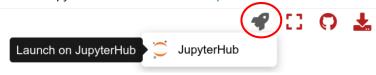


- Exercises account for 1/3 of the final grade (2/3 from exams, 1 written 1 oral)
- Submit report
 - pdf document answering the questions completely with relevant results
 - Handwritten portions ok (please verify legibility)
 - We provide report templates on Overleaf and Google Docs
 - Due date is usually the next exercise session (check Moodle!)
 - Interviews during next exercise session
 - Test your understanding and discuss your doubts/questions
 - Detailed feedback via Moodle after the interview



Computer environment

- We will use a virtual environment that you can directly launch from the exercise website
- Click the rocket button on the top right of the code files and choose JupyterHub to launch noto.epfl.ch



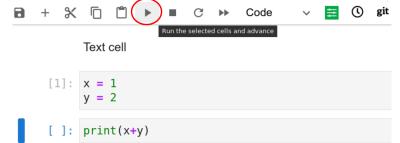
- On noto.epfl.ch your work will be saved on your EPFL storage
- Make sure to always activate (top right) the Computational Chemistry kernel





Jupyter notebooks

- .iynb files organized in cells
 - Markdown (text)
 - Code
- Run a code cell by pressing Play button (or Ctrl+Enter)



Exercise Session 1

Jupyter notebooks

- .iynb files organized in cells
 - Markdown (text)
 - Code
- Run a code cell by pressing :arrow_forward: (or Ctrl+Enter)



Text cell

```
[1]: x = 1
 y = 2
```



Linear Algebra in Quantum Mechanics - Exercise page

- Linear Algebra in Quantum Mechanics
- Basic Concepts in Quantum Mechanics
- Working with vectors using Numpy





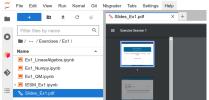
Exercise 1 - Tips

Tips!

- Start from Section 1.3 Working with vectos using Numpy to get familiar with Noto environment and Jupyter Notebooks
- How to get the slides:
 - Download from the exercise page



Once you open Noto, in the exercise folder



Will be uploaded on the Moodle page



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Exercise 1 - Tips

 We provide templates for the exercise reports, you can access them from the exercise page

```
Report Template Google Docs

Report Template Overleaf
```

- The answers can be short, for a full mark we don't expect more than what is explicitly asked
- You can ask for help anytime on the exercises and also the theory!
 - During the exercise session
 - During the week, on the Moodle Forum (public, so everyone can benefit from the answers and in principle you can help each other!)
 - At least one of us will be always present at the lectures, you can ask us questions before/after or during the break



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Exercise Sessions - Important Information

- The final grade from the exercises will be given by the best 8 out of 9 exercises. Hence in principle, you have a "free" exercise that you can decide to skip
- We will send a schedule for the interviews before each exercise session
- Please let us know in advance if you will not be able to be there for the interview
- In case of overlaps with other courses, we can schedule interviews also outside the exercise hours
- In case you don't show up at the interview and you don't contact us via email to reschedule the interview, the grade for that report will be 0