

# 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:
  - Yuri Cho
  - Salomé Guilbert
  - Sophia Johnson
  - Andrea Levy
  - Víctor Sabanza Gil
  - Qihao Zhang
  - Different PostDocs from LCBC lab

# Introduction to Electronic Structure Methods

- Mondays and Tuesdays from 10h15 to 12h00
- Course schedule for the semester available on Moodle and the exercise webpage
- Tomorrow we'll have the first lecture (in BCH3303) with more practical details on the course

- Moodle page



The screenshot shows the EPFL Moodle interface. At the top, there is a red vertical bar with a white right-pointing arrow, followed by the EPFL logo and the word 'MOODLE'. To the right, there are links for 'FR' and 'EN', and icons for a bell and a speech bubble. Below this header, the main title 'Introduction to electronic structure methods' is displayed in a large, bold, black font. Underneath the title, a breadcrumb trail reads: 'Dashboard > Courses > Chimie, Génie Chimique (CGC) > CGC - Bachelor > CH-353'.

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



# Exercise structure

## Introduction

- Learning goals
- Chapter in script
- Resources

 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:

## Exercise 9

Give the commutator of the position and linear momentum operators in the position representation (consider one dimension only).

## Bonus Exercise 10

Show that the potential energy operator  $\hat{V}(\mathbf{r})$  is multiplicative when applied to the real-space wavefunction.

*# Check Orthogonality*

```
 $\phi_1\phi_2 = 0$  # Replace with vector operation  
print(f'< $\phi_1|\phi_2$ > = { $\phi_1\phi_2$ }')
```

- Exercises account for 1/3 of the final grade (2/3 from two written exams)
- 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](https://noto.epfl.ch)



- On [noto.epfl.ch](https://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

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



Text cell

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

```
[ ]: print(x+y)
```

# Jupyter notebooks

- .ipynb 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
```

```
[3]: print(x+y)
```

3

# Exercise 1 - Overview

## Linear Algebra in Quantum Mechanics - [Exercise page](#)

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

### Learning goals

Review basic concept of linear algebra

Review basic notation of quantum mechanics

### Chapter in script

Chapter 2 - Basic principles of Quantum Mechanics

Appendix A.1 - Vector space and scalar product

### Resources

Cohen-Tannoudji, C., Diu, B., & Laloe, F. (1986). Quantum Mechanics, Volume 1.

- Chapter II B - State space, Dirac notation
- Chapter II C - Representations in the state space
- Chapter II D - Eigenvalue equations, observables
- Chapter II E - Two important examples of representations and observables
- Chapter II Complement D<sub>II</sub> - A more detailed study of the  $\{|r\rangle\}$  and  $\{|p\rangle\}$  representations
- Chapter II Complement E<sub>II</sub> - Some general properties of two observables,  $Q$  and  $P$ , whose commutator is equal to  $i\hbar$

# 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](#)

## 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

## 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