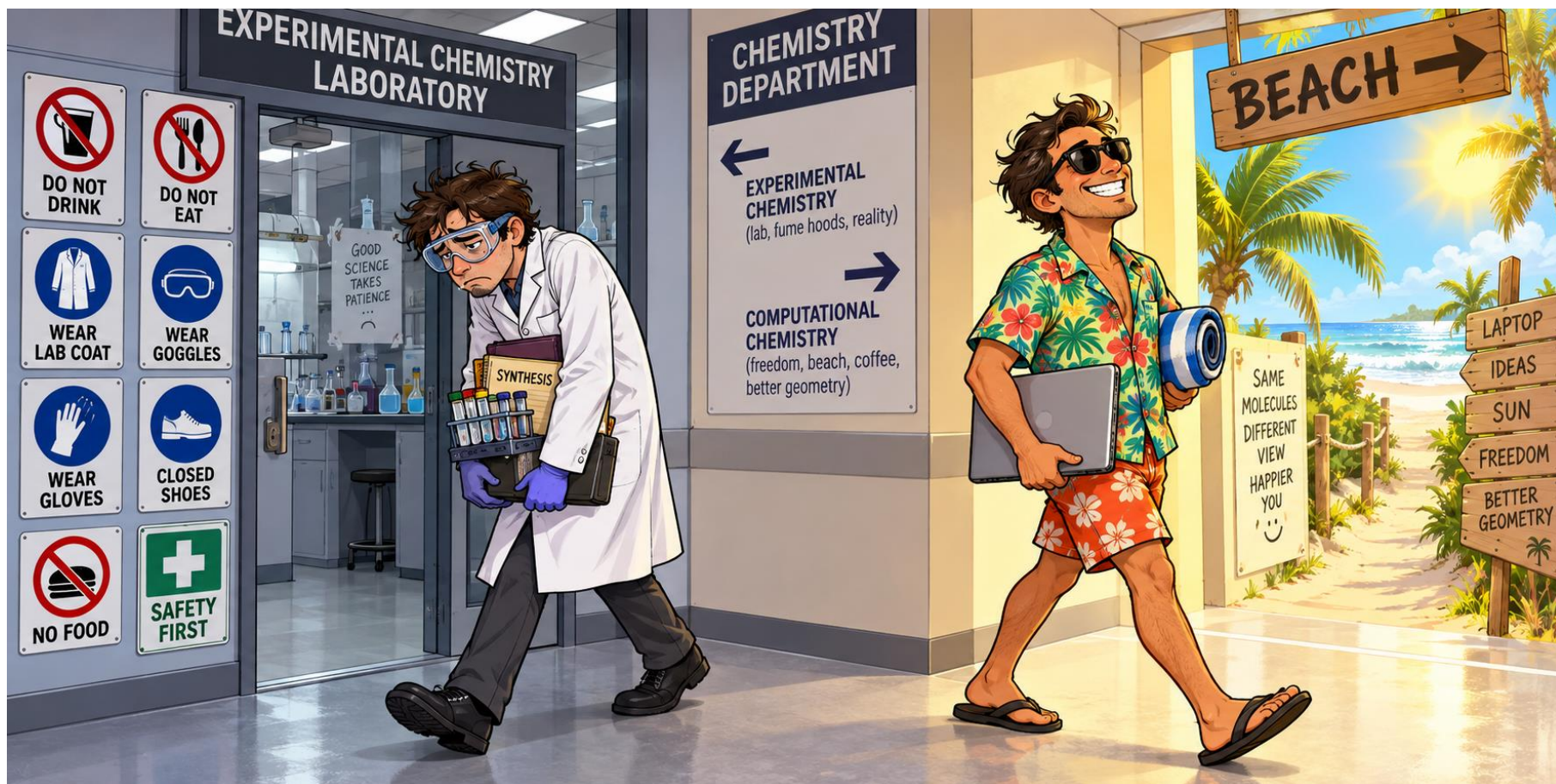


Materials design and selection for circular economy

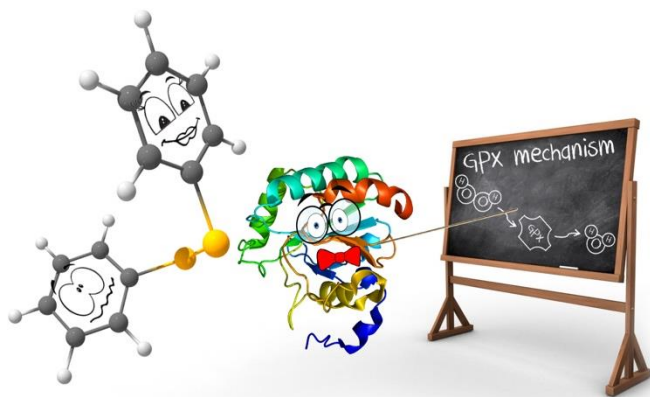
Mod. 2 Design and selection of functional molecules and materials
for sustainable synthesis and circularity

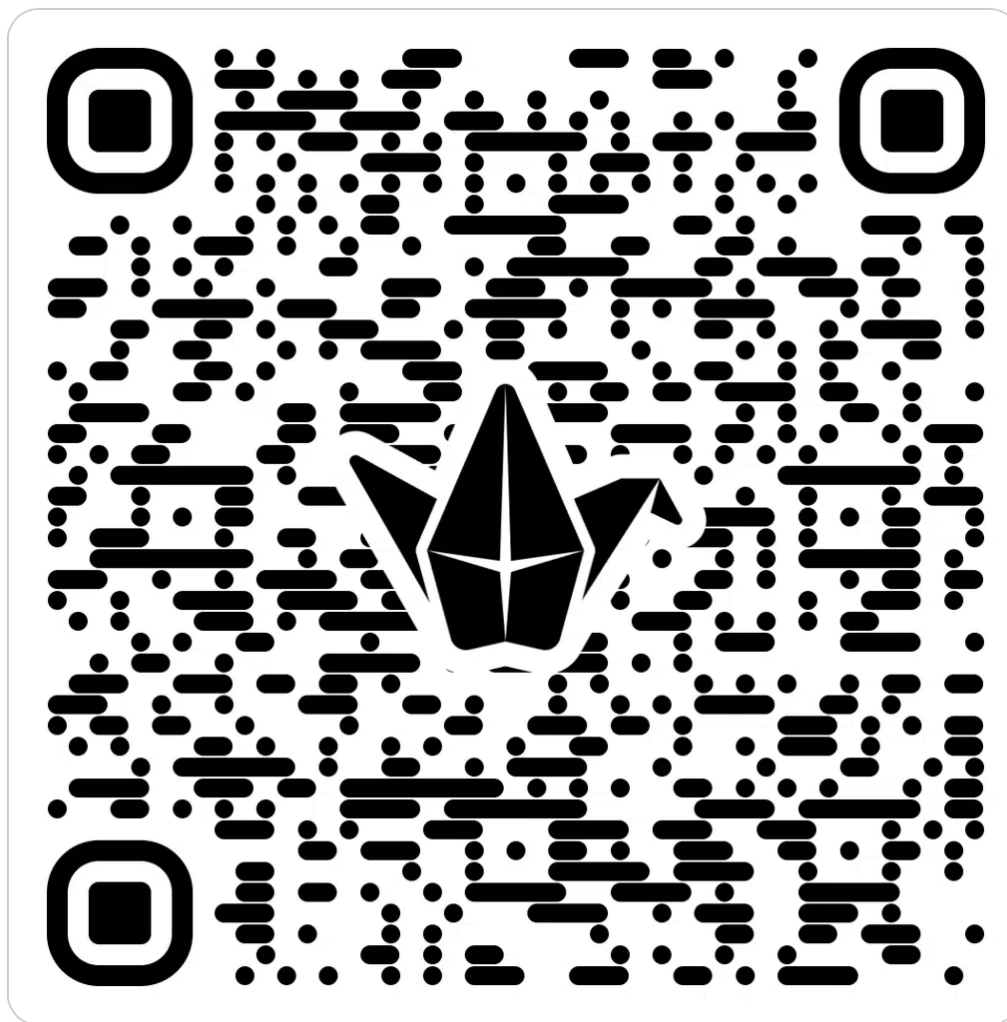
Laura Orian
DiSC UNIPD Via Marzolo 1 35131 Padova (IT)
laura.orian@unipd.it



More about ourselves....

We are all invited to post
our padlet sharing infos
about our interests,
background and a
photo...





laura.orian@unipd.it

- **Meeting**: e-mail booking: I will answer within 48 hours
- **Location**
DiSC Via Marzolo 1
or
ZOOM platform
- **Schedule**: upon agreement



What do you need?

1) **Exercise book:** *for notes and exercises*

2) **Calculator**

3) **BYOD:** *Bring Your Own Device (smartphone/laptop/tablet) to learn all together*

4) Link to **Moodle:**

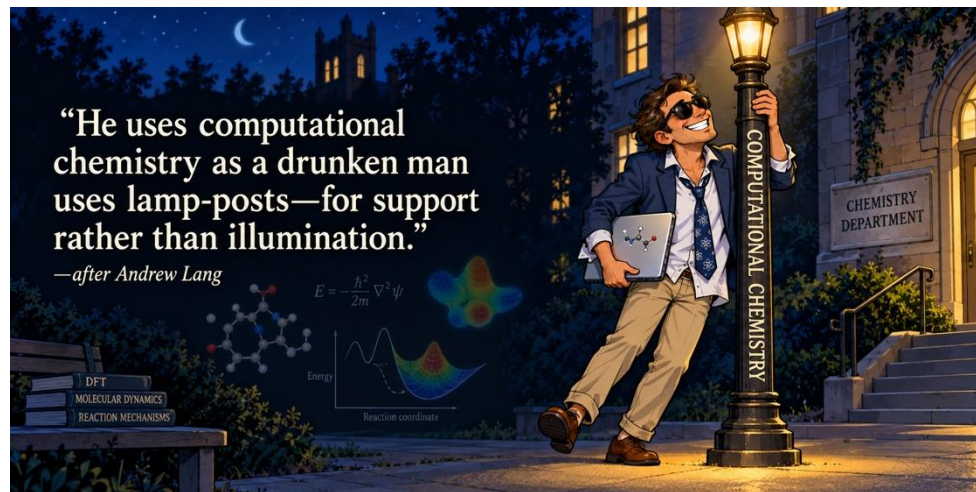
[Modifica corso: MATERIALS DESIGN AND SELECTION FOR CIRCULAR ECONOMY 2024-2025 - SCQ1095699 | STEM \(unipd.it\)](#)

From the syllabus...

The main goal of the module is to illustrate *how to design in silico a circular product and assess its physico-chemical properties.*

This approach requires the *introduction of the fundamentals and applications of few topics of computational chemistry to predict and interpret structural and reactivity properties of functional molecules and materials.*

1 ECTS devoted to **computational laboratory activity and description of case-studies.**



Some individuals use COMPUTATIONAL RESULTS as a drunk man uses lamp-posts — for support rather than for illumination.

Adapted from A. E. Housman (1903)

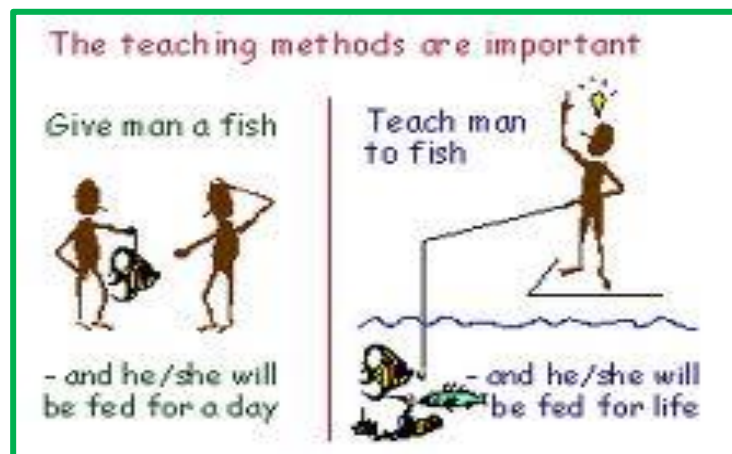
At the end of the course you'll be able to...

- Use a language adequate to describe modeling of chemical phenomena.
- Read and understand modeling aspects of chemical phenomena as described in literature.
- Execute basic QM calculations and understand their outputs.
- Attending a scientific seminar reporting on computational work



Teaching methods

- Interactive sessions in the class and discussion
- Group activities
- Short group presentations
- Use of technological tools; particularly, see the file: **Software for Chemistry.pdf**



Final examination

Please refer to the instructions provided by Prof. Gross at the beginning of the course.

The practical activity will be evaluated.

And now... let's finally **start this course!**

