

Venue

Department of Chemistry,
University of Coimbra (Portugal)

Lectures

Seminar Room (2nd floor)

Hands-on Sessions: Computer Room (1st floor)

How to reach the school venue

1. Arriving by plane



- From Lisbon Airport to Oriente train/bus station:
Metro red line (3 stops)
- From Porto Airport to Campanhã train/bus station:
Metro purple line (19 stops)

2. From Oriente/Campanhã to Coimbra



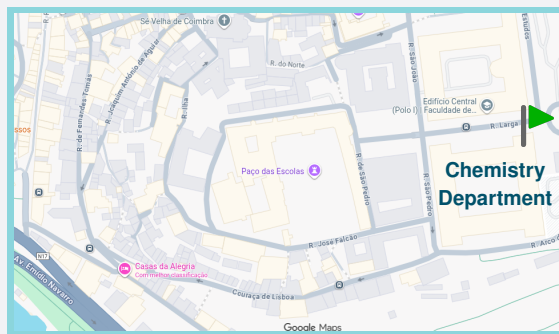
- Train: CP (<https://www.cp.pt/pt>)
- Bus: Rede Expressos (<https://rede-expressos.pt/pt>)
Flixbus (<https://www.flixbus.pt/>)

Note: Some buses depart directly from the airport to Coimbra (skip 1)

3. To Chemistry Department



- Uber/Bolt/Taxi
- Bus (<https://www.smtuc.pt/>):
Line 28 (stops at the Chemistry Department)
Line 5 (stops at 5 minutes walk from the University)



Local Organizing Committee

Jorge Marques

Joana Santos

Paulo Abreu

Tânia Cova

Scientific Committee

María Pilar de Lara-Castells, Spain

Francesca Mocci, Italy

Berta Fernández Rodríguez, Spain

Alberto Canelas Pais, Portugal

Contact

Jorge Marques

Department of Chemistry

University of Coimbra

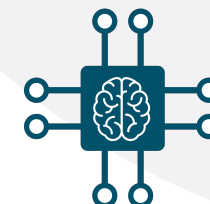


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Modeling

Potential Energy Functions with Machine Learning and Classical Techniques

COST CA21101 "COSY" Training School



University of Coimbra, Coimbra, Portugal
22st - 23rd January 2026



Training School

The program will include invited lectures and hands-on sessions on machine learning (ML) and computational chemistry, with open-source tools. This School aims to bring together PhD candidates and young researchers with expert trainers, mainly in the field of ML applied to computational chemistry.

The focus is on force field parameterization for molecular simulations using classical and ML-based approaches, with particular emphasis in force fields with interest in biological systems and materials.

Speakers

Saulo Vázquez, Spain

Francisco Pereira, Portugal

Markus Meuwly, Switzerland

Mandy Hoffmann, UK

Thantip Roongcharoen, Italy

Registration

CV (1 page maximum)

Motivation letter (1 page maximum)

Maximum 20 trainees

Reimbursement

16 trainees will be reimbursed

- 100 EUR of daily alloccance

- Up to 400 EUR for travel expenses

Programme

Wednesday, Jan 21

17:00-19:00 Registration/Informal visit to the Old University

Thursday, Jan 22

08:45-09:00 Opening Session/Late registration

09:00-11:00 Lecture/Hands-on session: Saulo Vázquez

11:00-11:30 Coffee Break

11:30-13:00 Lecture/Hands-on session: Francisco Pereira

13:00-14:30 Lunch

14:30-16:00 Lecture/Hands-on session: Markus Meuwly

16:00-16:30 Coffee Break

16:30-18:30 Lecture/Hands-on session: Thantip Roongcharoen

Friday, Jan 23

09:00-11:00 Lecture/Hands-on session: Mandy Hoffmann & Isaac Parker

11:00-11:30 Coffee Break

11:30-13:00 Lecture/Hands-on session: Mandy Hoffmann & Isaac Parker

13:00-14:30 Lunch

14:30-16:00 Hands-on session: Mandy Hoffmann & Isaac Parker

16:00-16:30 Coffee Break

16:30-18:00 Hands-on session: Omar Rodriguez

18:00-18:15 Closing remarks