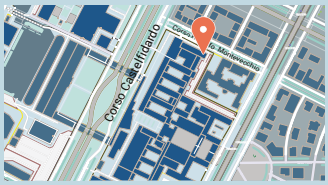
Lecturers: **Umberto Raucci** (IIT) & **Francesco Mambretti** (IIT)

1st class: MULTIMEDIA Meeting Room
DENERG North (second floor)
Corso Duca degli Abruzzi, 24
10138 Torino (TO)



class: **12th-13th-14th Nov 2025**
corse duration 9h

To enroll please contact:
matteo.fasano@polito.it

DENERG | Eccellenza 2023-2027 | Corso Breve

Atomistic simulations for energy related materials with machine learning-based interatomic potentials

The need for efficient energy storage and clean energy sources like hydrogen is increasing, driving the importance of **characterization of materials at the atomistic scale**, which is crucial to enhancing performance, particularly under operando conditions. Experimental characterization at atomic resolution is challenging yet crucial, while *ab initio* atomistic simulations offer a theoretical alternative to studying atomic-scale dynamics. However, the high cost of *ab initio* molecular dynamics restricts its use in realistic systems. **Recently, machine learning (ML)-based interatomic potentials have provided a practical way to balance *ab initio* accuracy with classical force field efficiency**. These ML potentials, trained on extensive quantum mechanical data, allow for simulations of larger systems over longer times. However, despite its power, constructing these potentials represents a complex endeavor.

This PhD course for Engineering students, even those with minimal molecular simulations knowledge, offers a comprehensive overview of the current state-of-theart methodologies in the field. We will discuss training ML potentials, collecting necessary data, and the pros and cons of each method. Additionally, **the course will feature illustrative applications to deepen participants' understanding** of structural dynamics, chemical kinetics, and transport phenomena in energy systems, focusing on specific examples like temperature effects on cathode materials and catalyst-involved chemical reactions.

The **hands-on section** will cover the complete training of a ML potential through case studies using Quantum Espresso (QE), DeepMD-Kit, MACE, LAMMPS, and Python.

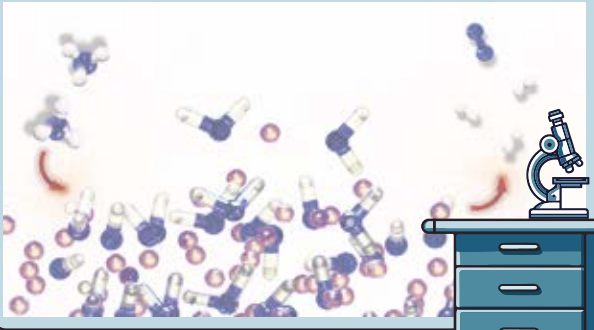
SILLABUS

- *Ab initio* & Classical Molecular Dynamics
- Enhanced Sampling
- Computing properties from Molecular Dynamics trajectories
- Temperature-induced lattice deformation in a cathode material
- Defects in Solid Electrolyte Interfaces
- Chemical reactions in presence of a catalyst

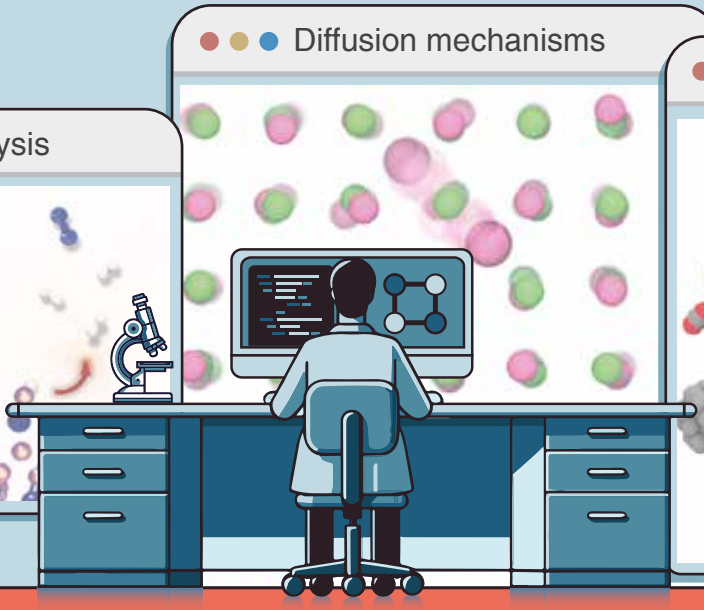
Umberto Raucci obtained his Ph.D in Chemical Science at the **University Federico II of Naples**. He is now a Postdoctoral Researcher in the **Atomistic Simulations group led by Prof. Parrinello** at the **Italian Institute of Technology**, where he moved after a post doctoral ex-perience in the **Martínez group** at the **Stanford University**. Umberto develops and applies theoretical methods to discover new chemical reactions in complex environ-ments using enhanced sampling techniques and machine learning based interatomic potentials.

Francesco Mambretti is a physicist and works as Postdoctoral Researcher in the **Atomistic Simulations group**, at the **Italian Institute of Technology**, in Genova. He is expert in Molecular Dynamics, Machine Learning and ab-initio simulations. His current research focuses on the study of **catalytic reactions for hydrogen production** and for graphene growth.

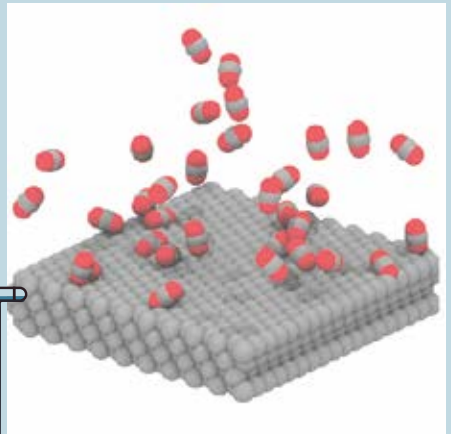
Heterogeneous Catalysis



Diffusion mechanisms



Interfacial properties



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