

# Irene Pusceddu – Curriculum Vitae

PhD Student in Computational Chemistry at Chimie ParisTech

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## Summary

I am a PhD Student at Chimie ParisTech - PSL in the Chemical Theory and Modelling group. My research experience spans modeling excited states, multiscale phenomena, and reactivity studies, with a consistent collaboration with experimental teams. I am deeply interested in exploring innovative computational methods and tackling complex chemical challenges to advance the field.

## Academic Background

**PhD Physical Chemistry**, Chimie ParisTech - PSL Sept 2024 - Ongoing

- Thesis: 'Multiscale modeling of mechanochromic systems' | Supervisor: Prof. Carlo Adamo

**Double Degree in Chemical Sciences**, Chimie ParisTech - PSL & University of Florence Sept 2021 - Jul 2024

- Final degree mark: High Honours - 110/110 cum laude
- M1 track in University of Florence: 'Structure, Dynamics and Reactivity'
- M2 track in Chimie ParisTech - PSL: 'Integrative Chemistry and Innovation'
- Thesis: 'A study of the optical properties of bio-source dyes.' | Supervisors: Prof. Marco Pagliari, Prof. Carlo Adamo and Prof. Ilaria Ciofini

**B.Sc. Chemistry**, University of Cagliari Sept 2018 - Jul 2021

- Final degree mark: 110/110 cum laude
- Thesis: 'Optical and structural characterization of ZnS/CaZnOS:Tb and CaZnOS:Tb' | Supervisor: Prof. Pier Carlo Ricci

## Professional Experiences

**PhD Physical Chemistry**, Chimie ParisTech - PSL Sept 2024 - Ongoing

- Development of a robust computational protocol to describe the phenomenon of mechanochromism in systems composed of dyes in polymer matrices.
- Financed by European Research Council (ERC) Advanced Grant

**Double Degree Internship**, Chimie ParisTech - PSL Feb 2024 – Jun 2024

- DFT and TD-DFT studies of the optical properties of perylene dimers. Molecular Mechanics simulations of perylene dimers in a polymer matrix. Hybrid particle-field coarse grained simulations of polymer matrices.

**Master Internship**, Chimie ParisTech - PSL Feb 2023 – Jun 2023

- Screening of the optical properties of a large set of bio-sourced dyes, conducted employing a computational protocol involving TD-DFT and DFT.

**Bachelor Internship**, Department of Physics, University of Cagliari Mar 2021 – Jun 2021

- Structural characterization of ZnS/CaZnOS:Tb and CaZnOS:Tb using Raman and XRD. Static and time-resolved measurements. Development of a new method of synthesis that leads to lower costs and environmental impact.

## Skills

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### Technological Skills:

- Programming Languages: **Bash, Python**
- Modeling Packages: **Gaussian, LAMMPS, OCCAM, NCIPLOT**
- Visualization Tools: **VMD, GaussView, CYLView**
- Data analysis softwares: **Excel, OriginLab**
- OS: **Linux (Ubuntu), Windows, MacOS**
- Text editors: **VIM, Word, EMACS, LaTeX**
- Machine Learning Packages: **scikit-learn**
- Presentation Tools: **LaTeX, PowerPoint**

### Soft Skills:

- Languages:
  - English** (Full proficiency)
  - Italian** (Mothertongue)
  - French** (Intermediate)
  - Spanish** (Intermediate)

## Fellowships

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### ERASMUS+ scholarship

Feb 2024 - Jun 2024

Università degli Studi di Firenze, Scuola di Scienze Matematiche, Fisiche e Naturali  
Scholarship for the international mobility of university students

### ERASMUS+ TRAINEESHIP scholarship

Feb 2023 - Jul 2023

Università degli Studi di Firenze, Scuola di Scienze Matematiche, Fisiche e Naturali  
Scholarship for the international mobility of university students

## Research Stays

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### University of Naples, Italy

14 - 30 Apr 2024

Short study visit with Prof. Giuseppe Milano

### Technische Universität Dresden, Germany

18 - 22 Nov 2024

Short study visit with Prof. Thomas Heine

## Conferences

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### DFT2024, Paris

25 - 30 Aug 2024

Poster Presentation: Pusceddu, I., Pagliai, M., Adamo, C., Cardini, G., and Ciofini, I. 'A study of the optical properties of a bio-sourced dye.'

## Teaching Experience

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**Supervision of internship - chemical engineer student**, Chimie ParisTech - PSL

Nov 2024 - Ongoing

**Supervision of internship - chemical engineer student**, Chimie ParisTech - PSL

Mar 2023 - Jul 2023

## Extracurricular Activities

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### Rotary Youth Exchange Participant

Aug 2016 - Jul 2017

- Engaged in a year-long cultural immersion program in Kamloops BC, Canada
- Represented Italy as a cultural ambassador
- Gave presentations on Italian and Sardinian culture to local communities
- Developed fluency in English and enhanced cross-cultural communication and leadership skills

### Mentee - PSL Femmes & Sciences Mentorship Program

Jan 2025 - Ongoing

- 11 workshops and trainings
- 1 individual meeting with the mentor per month