Pablo **Grobas Illobre**

Spanish 10/10/1996

Computational Chemist

Scientific Software Developer

Profile Summary

Computational chemist and **scientific software developer** with **6+ years'** experience in **computational modeling, QM/MM, and HPC workflows.** Skilled in **C++/Fortran/Python** programming with a proven track record in **scientific software development** and international collaborations. **Currently transitioning** toward the **drug discovery industry**, applying **physics-based ML** and high-performance computing to molecular modeling challenges.

Contact Details

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github.com/pgrobasillobre
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Languages

- Spanish (native)
- Galician (native)
- English (fluent)
- Italian (fluent)
- French (fluent)

Technical Skills

- **Programming Languages**: Python, C++, Fortran, Matlab
- **Python Libraries**: NumPy, SciPy, Matplotlib, TensorFlow, PyTorch, Scikit-learn, Keras
- **Fortran Development**: OpenMP parallelization, CMake compilation
- **Development Tools**: Git, Visual Studio Code, Vim
- **Operating Systems and Scripting**: Proficient in Linux and Bash/shell scripting
- **Interactive Environments**: Jupyter, Google Colab
- **Scientific Software**: Amsterdam Modeling Suite, Gaussian
- **High Performance Computing (HPC) environments**

Experience and Training

Postdoctoral Researcher,
Scuola Normale Superiore | 02/2025 - Present | Pisa, Italy

Currently developing **QM/MM quantum chemistry software** in **C++** and **Fortran** in collaboration with the *Software for Chemistry & Materials* company. This work is complemented by **Python programming** for **machine learning**, **data analysis**, **statistics**, and **visualization**.

My research integrates intensive **software development** to investigate:

- **QM/MM Surface-Enhanced Spectroscopies**: Fluorescence, Raman scattering, Raman optical activity.
- **Plasmonic Materials**: graphene & metal nanoparticles.
- **Plasmon Mediated Electronic Energy Transfer**.

Ph.D. (*cum laude*) in Methods and Models for Molecular Sciences,
Scuola Normale Superiore | 11/2020 – 01/2025 | Pisa, Italy

Title: Modeling Atomistic Nanoplasmonics: Classical and Hybrid Quantum Mechanical/Classical Schemes

Supervisor: Chiara Cappelli

M.Sc. in Theoretical Chemistry and Computational Modeling,
Université Paul Sabatier | 09/2018 – 08/2020 | Toulouse, France

M.Sc. Thesis, *University of Trieste*
11/2019 – 08/2020 | Trieste, Italy

Fortran software development for quantum chemistry

Visiting Student, *Autonomous University of Madrid*
09/2019 - 10/2019 | Madrid, Spain

M.Sc. Internship, *Okayama University*
04/2019 - 06/2019 | Okayama, Japan

Molecular dynamics simulations of ions in solution.

Research Assistant, *Instituto de Tecnología Química*
07/2019 – 08/2019 | Valencia, Spain

Molecular dynamics for sugar separation in the food industry.

Supervisor: Germán Ignacio Sastre Navarro

B.Sc. in Chemistry, *University of A Coruña*
09/2014 – 07/2018 | A Coruña, Spain

Erasmus Exchange, *University of Oslo* | 08/2016 - 12/2016

Research Projects

GEMS - General Embedding Models for Spectroscopy, *ERC Consolidator Grant*

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- **Python** programming (in-house codes) for **data analysis**, **manipulation**, and **visualization** (e.g., see examples of Python-driven figures in T. Giovannini *et al.*, *ACS Photonics*, 2022, 9, 3025).
- Currently developing a **machine learning** pipeline in **Python** to study and simulate graphene samples.
- Quantum chemistry **software development** in **Fortran** (within the Amsterdam Modeling Suite and in-house codes) for modeling plasmonic materials, **QM/MM** surface-enhanced Raman scattering, and Raman optical activity.
- Intensive use of **HPC** infrastructures to streamline large-scale **data production** workflows.

FARE - "Framework per l'attrazione e il rafforzamento delle eccellenze per la ricerca in Italia"

Scuola Normale Superiore | 2020 - 2025 | PI: Chiara Cappelli

- **Python** programming (in-house codes) for **data analysis**, **manipulation**, and **visualization** (e.g., see generated Python-driven figures in P. Grobas Illobre, *et al.*, *Nanoscale Adv.*, 2024, 6, 3410).
- Quantum chemistry **QM/MM software development** in **C++** and **Fortran** (within the Amsterdam Modeling Suite and in-house codes) for modeling surface-enhanced fluorescence, and plasmon-mediated electronic energy transfer.
- Intensive use of **HPC** infrastructures to automate and streamline **data production** workflows.

Selected Publications

- **P. Grobas Illobre**, P. Lafiosca, T. Guidone, F. Mazza, T. Giovannini, C. Cappelli, "Multiscale Modeling of Surface Enhanced Fluorescence", *Nanoscale Adv.*, 2024, **6**, 3410.
- **P. Grobas Illobre**, P. Lafiosca, L. Bonatti, T. Giovannini, C. Cappelli, "Mixed atomistic–implicit quantum/classical approach to molecular nanoplasmonics", *J. Chem. Phys.*, 2025, **162**, 044103.

Supervision & Teaching

B.Sc. Thesis: "Fluorescence Response of Chromophores Near Plasmonic Nanoparticles: Atomistic vs. Continuum Approaches" – Teresa Guidone (2023), *Scuola Normale Superiore*

I supervised B.Sc. student Teresa Guidone for her thesis project, which included:

- Reviewing scientific literature in quantum chemistry, specifically on surface-enhanced fluorescence.
- Teaching Fortran95 (including parallelization) and Python programming.
- Guiding Fortran95 algorithm design, implementation, and debugging in the Amsterdam Modeling Suite.
- Leading Python data analysis and manipulation.
- Instructing in the use of Linux and High-Performance Computing (HPC) environments.

Course Teaching: Advanced Topics in Quantum Chemistry (2024), *Scuola Normale Superiore*

I delivered practical sessions in quantum chemistry for Ph.D. and master's students, which included:

- Teaching various energy decomposition methods within quantum chemistry.
- Organizing hands-on sessions with the GAMESS quantum chemistry software.
- Training in Linux and HPC environment usage.
- Providing guidance on data generation and analysis.

Awards

- PhD awarded with honors (*cum laude*)
- Scuola Normale Superiore PhD Scholarship (2020-2025).
- Two NanoX Research Scholarships (2019 & 2020).
- Erasmus Internship Fellowship (2019-2020).
- Consejo Superior de Investigaciones Científicas (CSIC) – Jae Intro Fellowship (2019).
- Extraordinary Prize for achieving the best academic record in the Bachelor of Chemistry (2018).
- Erasmus+ scholarship (2016).