

ABBREVIATED CURRICULUM VITAE

Part A. PERSONAL INFORMATION

Name and Surnames	Diego Ontiveros Cruz		
DNI/NIE/passport	25369712E		
e-mail	diegonti.doc@gmail.com	Phone	+34 644311635
Researcher identification IDs	Researcher ID	IST-1983-2023	
	OrcID	0009-0008-0307-5645	

Part B. SUMMARY

I hold a degree in Chemistry from the University of Barcelona, and I further expanded my knowledge by completing a master's degree in Computational Modeling. My research experience primarily focuses on projects involving the computational study of materials and their application as photocatalysts. I possess extensive programming skills, enabling me to optimize and automate calculation processes and result analysis through Python scripts. I am a dedicated individual, eager to learn, collaborate, and continually improve. I am organized, ambitious, and capable of working both independently and as part of a team. My passion lies in computational chemistry, which I aim to pursue in the coming years, as well as in the field of scientific outreach.

Part C. ACADEMIC INFORMATION AND MERITS

◆ Studies and academic degrees

- **Master's Degree in Atomistic and Multiscale Computational Modelling.** University of Barcelona, 2022–2023. Grade: 9.3/10.0
- **Bachelor's Degree in Chemistry.** University of Barcelona, 2018–2022. Grade: 8.4/10.0

◆ Research activity, including grants, scholarships and research contracts and participation in projects and agreements

- **PREDOCS-UB predoctoral contract.** March 2024 – March 2027.
- **Grant for the PhD Initiation** in the Faculty of Chemistry. November 2023 – February 2024.
- **Collaboration Fellowship** with the Material Science and Physical Chemistry Department. November 2022 – June 2023.
- **Càtedra UB Fellowship** - Fundación Privada José Luis Massó – Grant for enrollment in university masters at the Faculty of Chemistry of the UB. October 2022.

◆ Publications (articles, book chapters and others)

- **Exploring the Photoactive Properties of Promising MXenes for Water Splitting**
D. Ontiveros, F. Viñes, C. Sousa. *J. Mater. Chem. A*, 2025, **13**, 3302–3316. DOI: [10.1039/D4TA06852A](https://doi.org/10.1039/D4TA06852A)
- **Tuning MXenes towards their Use in Photocatalytic Water Splitting**
D. Ontiveros, S. Vela, F. Viñes, C. Sousa. *Energy Environ. Mater.*, 2024, e12774. DOI: [10.1002/eam2.12774](https://doi.org/10.1002/eam2.12774)
- **Bandgap Engineering of MXene Compounds for Water Splitting**
D. Ontiveros, F. Viñes, C. Sousa. *J. Mater. Chem. A*, 2023, **11**, 13754–13764. DOI: [10.1039/D3TA01933K](https://doi.org/10.1039/D3TA01933K)

- **Bandgap Engineering on MXene Compounds by Structure, Composition, and Surface Termination**
D. Ontiveros. Dipòsit Digital UB, TFG. hdl.handle.net/2445/189371

♦ Participation in congresses and conferences

- **Exploring the Photoactive Properties of MXenes for Water Splitting** – Flash Presentation + Poster
2^a Reunió de Química Teòrica i Computacional (RQTC-SCQ), Barcelona, 2025 ([Link](#)).
Awarded best flash presentation.
- **Exploring the Photoactive Properties of MXenes for Water Splitting** – Poster
Twins in Catalysis Symposium, Barcelona, 2024 ([Link](#)).
- **Exploring the Photoactive Properties of MXenes for Water Splitting** – Poster
IQTC/QTMC Meeting 2024, UB, 2024 ([Link](#)).
- **Computational Study of MXenes for Water Splitting Photocatalysis** – Flash Presentation
EUROMXENE Congress, Valencia, 2024 ([Link](#)).
- **MXenes as Photocatalytic Materials for Water Splitting** – Poster
IQTC/QTMC Meeting 2023, UB, 2023 ([Link](#)).
- **Computational Study of MXenes as Photocatalytic Materials** – Flash Presentation + Poster
8th International Conference on Semiconductor Photochemistry (SP8), Strasbourg, 2023 ([Link](#)). Awarded best flash presentation.
- **MXens com a Fotocatalitzadors del Trencament de l'Aigua** – Poster
Masterquímica XVIII, Committee for Linguistic Dinamization, UB, 2023 ([Link](#)).

♦ Participation in workshops or courses

- VASP **workshop** - From setup to solution, Online, 2024
- Quantum Computing **Masterclass**, Quantum Spain & BSC, Barcelona, 2023.
- IQTC **Course** - Computational Modelling: from Molecules to Materials, Barcelona, 2022.
- IQTC **Course** - Molecular Modelling: biomolecules and drug design, Barcelona, 2023.

♦ Science communication activities

- My **personal web page** with more academic and projects information: diegonti.github.io
- My **networks** where I update my activity as a research scientist (ResearchGate, LinkedIn, Google Scholar, ORCID): linktr.ee/diegonti
- **Scientific disseminator** for secondary school with [IQTC Talks](#). 2024.
- **Dissemination videos** of my research in the [CMSLUB](#) YouTube Channel. 2024.
- **Scientific monitor** for workshops for children aged 7–14 at Smart Barcelona. 2023.
- **Educational support** teacher in the Èxit program. 2018–2020 and 2022.

- **Finalist in the 10th Young Research Exhibition** of Barcelona ([CEB](#)), 2018.

♦ **Other relevant academic and/or scientific merits, including awards, and recognitions**

- **6 Distinctions in the Chemistry Degree:**
Physics I (9.6), Basic Inorganic Lab (9.2), Organic Chemistry I (9.3), Organic Chemistry III (9.8), Structural and Spectroscopic Organic Chemistry (9.5), Final Degree Thesis (9.9).
- **5 Distinctions in Computational Modelling Master's Degree:**
Statistical Mechanics (9.5), Molecular Modelling (9.0), Electronic Structure (10), Electronic Structure in Solids (9.5), Nanomaterials and Surfaces Modelling (9.6).
- **B2 English** Level certified by Cambridge Assessment English (**Grade A** – Score 181).
- **Awarded the best Flash Oral Communication prize** at 2a Reunió de Química Teòrica i Computacional (RQTC-SCQ), Barcelona, 2025.
- **Awarded the best Flash Oral Communication prize** at 8th International Conference on Semiconductor Photochemistry (SP8), Strasbourg, 2023.
- Good knowledge of **Python** and programming tools. github.com/diegonti
- **Spanish** and **Catalan** as native languages.