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

  - **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/eem2.12774

  - **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

- **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**

- **MXgap: A MXene Learning Tool for Bandgap Prediction** – Poster
  World Association of Theoretical and Computational Chemists (WATOC), Oslo, 2025 (Link).

- **Exploring the Photoactive Properties of MXenes for Water Splitting** – Invited Talk
  VASP and Applications Online Conference, Évora, 2025 (Link).

- **Explorant les Propietats Fotoactives dels MXens per a la Divisió de l'Aigua** – Flash Presentation + Poster
  2ª 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.