ABBREVIATED CURRICULUM VITAE

Full name	Diego Ontiveros Cruz		
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Part A. SUMMARY

I hold a Bachelor's degree in Chemistry from the University of Barcelona and completed a Master's in Computational Modeling. I am currently pursuing a PhD in Computational Chemistry, with a research focus on the computational study of materials and their photocatalytic applications. I have strong programming skills, particularly in Python, which I use to optimize and automate simulations, analyze data, and develop machine learning models. My passion lies in advancing computational chemistry and contributing to scientific outreach efforts.

Part B. 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 2028.

- **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 master's at the Faculty of Chemistry of the UB. October 2022.

♦ **Publications**

- **MXgap: A MXene Learning Tool for Bandgap Prediction**
  D. Ontiveros, S. Vela, F. Viñes, C. Sousa. *ACS Catal.*, 2025, **15**, 14403–14413. DOI: 10.1021/acscatal.5c04191

- **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, **7**, 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
  IQTC/QTMC Meeting 2025, UB, 2025 (Link).

- **MXgap: A MXene Learning Tool for Bandgap Prediction** – Invited Talk
  COST CIG Conference on machine learning and multiscale modeling of nanocrystal catalysts, Budapest, 2025 (Link).

- **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). Assistance to the organization.

- **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**

- Initiation on Quantum Computing **Workshop**, IQTC & CSUC, Barcelona, 2025.

- 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 outreach** for secondary school with IQTC Talks. 2024.

- **Dissemination videos** of my research in the CMSLUB YouTube Channel. 2024.

- **Scientific monitor** in 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](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).

- **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.

- **Teaching assistant** (+60h) as part of the PhD contract.

- Proficient in **Python** and related programming tools. github.com/diegonti

- **B2 English** Level certified by Cambridge Assessment English (**Grade A** – Score 181).

- **Spanish** and **Catalan** as native languages.