

## CURRICULUM VITAE

Family name, First name: **DROSOU, Maria**

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Date of birth: August the 3<sup>rd</sup> 1994, Nationality: Greek

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Google Scholar: <https://scholar.google.gr/citations?user=pHYczhQAAAAJ&hl=en>

## RESEARCH INTERESTS

I use theoretical chemistry to investigate the electronic structure, magnetic and spectroscopic properties, reactivity, and photochemistry of (bio)molecular systems involved in energy conversion and catalysis. My research focuses on developing integrative computational approaches that combine methods ranging from high-level wave function-based methods to density functional theory and semiempirical calculations, and applying them to generate fundamental insights and concepts for designing new functional molecular systems. Research axes:

- bioinspired multinuclear transition metal catalysts for water oxidation,
- excited states of multichromophoric systems in Photosynthesis,
- computational protocol development for computational spectroscopy of transition metal complexes.

## EMPLOYMENT

- 10/2026–present CNRS researcher (CRCN), iSm2, Marseille, France
- 07/2025–09/2026 Junior Group Leader Liebig Fellow, Technische Universität Darmstadt, Germany
- 07/2023–06/2025 Humboldt Research Fellow, Max-Planck-Institut für Kohlenforschung, Germany  
Supervisor: D. A. Pantazis
- 04/2022–06/2023 Postdoctoral Researcher, Max-Planck-Institut für Kohlenforschung, Germany  
Supervisor: D. A. Pantazis

## SCIENTIFIC EDUCATION

- 2018–2022 Ph.D. in Inorganic Chemistry (with honors), University of Athens, Greece  
Supervisor: C. A. Mitsopoulou
- 2020 3-Month Research Internship, Max-Planck-Institut für Kohlenforschung, Germany  
Supervisor: D. A. Pantazis
- 2016–2018 M.Sc. in Inorganic Chemistry, University of Athens, Greece  
Supervisor: C. A. Mitsopoulou
- 2012–2016 Studies of Chemistry, University of Athens, Greece (with honors 8.62/10)  
Supervisor: C. A. Mitsopoulou

## RESEARCH FUNDING AND FELLOWSHIPS

- 2025 Liebig Fellowship, Fonds der Chemischen Industrie (2025) — competitive individual award, ≈ €250,000 (3 years)
- 2023
- Alexander von Humboldt Foundation's Scholarship for Postdocs (2 years)
  - German Academic Exchange Service (Deutscher Akademischer Austauschdienst, DAAD) Programme for Project-Related Personnel Exchange (PPP) from 2023 with France
- 2019 Hellenic Foundation for Research and Innovation Scholarship for Ph.D. in Greece (3 years)
- 2018 Onassis Foundation Scholarship for Ph.D. in Greece (3 years)

## HONORS AND AWARDS

- 2023 Ernst Haage Prize

- 2022 Quantum Bio-Inorganic Chemistry Society award for oral presentation in GDR Solar Fuels Réunion Annuelle, Nice, France
- 2017 M.Sc. honors with distinction and remission of registration fee
- 2012 Eurobank Scholarship for Excellence at National University Entrance Examinations — Top-ranked student at my high school

## PUBLICATIONS

**25** peer-reviewed publications (first author: **13**; corresponding author: **5**) in high-impact peer-reviewed international journals, including: *J. Am. Chem. Soc.* (3), *Angew. Chem.* (3), *J. Chem. Theory Comput.* (2), *JACS Au* (1), *Chem. Sci.* (1), *Inorg. Chem.* (2), *Chem. Eur. J.* (3). Google Scholar (updated 06/10/2026): h-index **13**, total number of citations: **582**.

**Selected publications:** (Publications as corresponding author are marked with an asterisk (\*))

1. \***Drosou, M.**, Bhattacharjee, S., Pantazis, D. A., Combined Multireference–Multiscale Approach to the Description of Photosynthetic Reaction Centers. *J. Chem. Theory Comput.* **2024**, 20(16), 7210–7226. [open access, <https://doi.org/10.1021/acs.jctc.4c00578>]
2. Chrysina, M., **Drosou, M.**, Castillo, R. G., Reus, M., Neese, F., Krewald, V., Pantazis, D. A., DeBeer, S., Nature of S-States in the Oxygen-Evolving Complex Resolved by High-Energy Resolution Fluorescence Detected X-ray Absorption Spectroscopy. *J. Am. Chem. Soc.* **2023**, 145(47), 25579–25594. [open access, <https://doi.org/10.1021/jacs.3c06046>]
3. **Drosou, M.**, Comas-Vilà, G., Neese, F., Salvador, P., Pantazis, D. A., Does serial femtosecond crystallography depict state-specific catalytic intermediates of the oxygen-evolving complex? *J. Am. Chem. Soc.* **2023**, 145(19), 10604–10621. [open access, <https://doi.org/10.1021/jacs.3c00489>]
4. \***Drosou, M.**, Mitsopoulou, C. A., Pantazis, D. A., Reconciling Local Coupled Cluster with Multireference Approaches for Transition Metal Spin-State Energetics. *J. Chem. Theory Comput.* **2022**, 18(6), 3538–3548. [open access, <https://doi.org/10.1021/acs.jctc.2c00265>, data available at the Open Research Data Repository of the Max Planck Society at <https://doi.org/10.17617/3.XWIA1R>]
5. **Drosou, M.**, Zahariou, G., Pantazis, D. A., Orientational Jahn–Teller Isomerism in the Dark-Stable State of Nature’s Water Oxidase. *Angew. Chem. Int. Ed.* **2021**, 60(24), 13493–13499. [open access, <https://doi.org/10.1002/ange.202103425>]

## CONFERENCE PRESENTATIONS

**27** oral contributions - **11** poster communications - **4** invited seminars and **4** invited talks.

Invited talks:

- 2026 2<sup>nd</sup> Symposium on Solar-Driven Chemistry (SOLCHEM), Ulm, Germany.
- 2026 19<sup>th</sup> Conference on Theory, Modelling, Simulation at the Atomic scale (TheMoSiA), Nantes, France.
- 2026 1<sup>st</sup> Danish-Hellenic Coordination Chemistry Conference (DH3C), Trikala, Greece.
- 2023 Ernst Haage Prize for Chemistry Award Ceremony, Mülheim an der Ruhr, Germany.

## SUPERVISION OF GRADUATE STUDENTS

**Supervision:** 1 Ph.D. student (currently), 1 Intern (defended). **Co-supervision:** 1 Ph.D., 2 Master’s students.

## TEACHING ACTIVITIES

- 2025:** Quantum Chemistry I and II (Master's level) at Technische Universität Darmstadt, Germany.
- 2023–2024:** Tutor and lecturer at Summer School “Spectroscopy and Electronic Structure of Transition Metal Complexes”, Max-Planck-Institut für Kohlenforschung, Germany, and at the Virtual Winter School on Computational Chemistry (VWSCC25).
- 2016–2018:** Tutor and Laboratory Instructor at Inorganic Chemistry laboratory exercises (Bachelor's level) at University of Athens, Greece.

## MEMBERSHIPS OF SCIENTIFIC SOCIETIES

- Since 2025: Theoretical Chemistry Working Group (Arbeitsgemeinschaft Theoretische Chemie, **AGTC**)
- Since 2024: International Society of Photosynthesis Research (**ISPR**)
- Since 2022: Quantum Bio-Inorganic Chemistry Society (**QBIC**)

## SERVICE TO THE COMMUNITY — PEER REVIEW

**12** peer-reviewed articles: *ACS. Catal.* (1), *Dalton Trans.* (3), *Inorg. Chem.* (1), *Nat. Commun.* (2), *Phys. Chem. Chem. Phys.* (3), *J. Phys. Chem. Lett.* (2).