

## 1. Personal Information and Current Position



- Dr. Carla Casadevall Serrano
- Date of birth: 07/06/1991 – Spain - Nationality: Spanish
- E-mail: [carla.casadevall@urv.cat](mailto:carla.casadevall@urv.cat), [ccasadevall@iciq.es](mailto:ccasadevall@iciq.es)
- Current position: Ramón y Cajal Fellow and Junior Group Leader at University Rovira i Virgili (URV) and Institute of Chemical Research of Catalonia (ICIQ), Tarragona (Spain): [https://www.iciq.org/research/research\\_group/dr-carla-casadevall/](https://www.iciq.org/research/research_group/dr-carla-casadevall/)
- Accredited as Lecturer by the Catalan Quality Agency (AQU).
- Google Scholar: [carla casadevall serrano](https://scholar.google.com/citations?user=carla_casadevall_serrano)
- Twitter: @CasadevallCarla
- Orcid: 0000-0002-3090-4938 - Researcher ID: A-5231-2019 - Scopus ID: 57190175910

## 2. Education

**2014-2019: International PhD in Chemical Science and Technology** (Excellent-Cum Laude, maximum distinction). Institute of Chemical Research of Catalonia (ICIQ) - University Rovira and Virgili (URV), Spain. **PhD Thesis title:** “*Mechanistic studies of water oxidation catalyzed by homogeneous iron and ruthenium complexes and light-driven organic reductions with a dual cobalt/copper catalytic system.*” Advisor.: Prof. Julio Lloret-Fillol.

**2013-2014: MSc Advanced Catalysis and Molecular Modelling** (9.5/10, best mark of my promotion, honor distinction). University of Girona (UdG), Spain. **MSc Project:** “*Unravelling the water oxidation mechanism of novel tacn-based ruthenium complexes.*” Advisors: Prof. Miquel Costas and Prof. Julio Lloret-Fillol.

**2009-2013: Bsc Chemistry** (9.3/10, best mark of my promotion, honor distinction) University of Girona (UdG), Spain.

**Bsc Project:** “*Synthesis of novel ruthenium complexes based on the Pytacn moiety and study of their catalytic activity in C-H bond and water oxidation.*” Advisors: Prof. Miquel Costas and Prof. Julio Lloret-Fillol.

## 3. Previous Positions and Research Experience

- 01/01/2023-present: Ramón y Cajal Fellow and Junior Group Leader at URV and ICIQ (Spain).
- 01/10/2022-31/12/2022: Junior Group Leader “La Caixa” and Associate Professor at ICIQ and URV (Spain).
- 01/10/2020-31/09/2022: Marie Curie Individual Fellow (ref: 890745, SmArtC) in the group Prof. E. Reisner at the University of Cambridge (UK).
- 12/09/2019-30/09/2020: BBSRC Postdoctoral Research Associate (ref: BB/S00159X/1) in the group Prof. E. Reisner at the University of Cambridge (UK).
- 23/07/2019-11/09/2019: Postdoctoral Research Associate in the group of J. Lloret-Fillol at ICIQ (ERC-2015-CoG-648304 contract, Spain).
- 01/01/2019-22/07/2019: Research associate (PhD student) in the group of Prof. J. Lloret-Fillol at ICIQ (ERC-2015-CoG-648304 contract, Spain).
- 01/09/2015-31/12/2018: FPU-PhD fellow (ref: FPU14/02550) in the group of Prof. J. Lloret-Fillol at ICIQ (Spain).
- 04/11/2014-31/08/2015: CELLEX-PhD fellow (ref: ICIQ-SCP) in the group of Prof. J. Lloret-Fillol at ICIQ (Spain).
- 01/10/2013-03/11/2014: Research assistant-master student in the group Prof. M. Costas (“Beca de colaboración” fellowship) at the University of Girona (Spain).
- 01/09/2012-30/09/2013: Research assistant – Chemistry degree project student in the group Prof. M. Costas (“Xavier Gironès” fellowship) at the University of Girona (Spain).

## 4. Teaching Experience

- 2023-2024: 1) Organometallic chemistry and homogeneous catalysis at the URV-ICIQ Master in synthesis, catalysis and molecular (18 h). 2) 1<sup>st</sup> year Chemistry degree Inorganic Chemistry lab (30 h).
- 2022-2023: 1) Organometallic chemistry and homogeneous catalysis at the URV-ICIQ Master in synthesis, catalysis and molecular (15 h).
- 2020-2021: 1<sup>st</sup> year and 2<sup>nd</sup> year Organic chemistry supervisions University of Cambridge (20 h).
- 2019-2020: 1<sup>st</sup> year Chemistry Supervisions, University of Cambridge (45 h).
- 2015–2018: 1<sup>st</sup> year Chemistry Lab, University Rovira i Virgili (60 ECTS / year).
- 2012–2013: 1st year Chemistry Supervisor, University of Girona (10 h).

## 5. Fellowships and Awards

- 2023: Emerging Scientific Talent Award (“Premi al Talent Científic Emergent”) from the Catalan Society of Chemistry (SCQ) for in recognition for the scientific trajectory and the emerging leadership.
- 2023: Young Investigator Award from the Spanish Royal Society of Chemistry (RSEQ).
- 2023: Best oral presentation in the 1<sup>st</sup> organometallic and inorganic chemistry meeting from the Catalan Chemical Society (SCQ) 2023.

- 2022: Ramon y Cajal Fellowship 2022, ref: RYC2021-030935-I.
- 2022: La Caixa Junior Leader Incoming Fellowship 2022, ref: LCF/BQ/PI22/11910020.
- 2021: Maria Zambrano Fellowship 2021 (from NextGenerationEU), ref: 2021URV-MZ-07.
- 2019: Marie Skłodowska-Curie Individual Fellowship 2019 (MSCA-IF-2019), ref: 890745-SmArtC, European Commission.
- 2018: Best experimental oral presentation at the Girona Seminar 2018 conference.
- 2015: CARISMA COST PhD Travel grant 2015, ref: EU COST ACTION CM1205.
- 2014: FPU PhD fellowship Spanish Ministry (most competitive PhD fellowship in Spain). Ref: FPU14/02550. Sept. 2015/Dec. 2018.
- 2014: CELLEX PhD fellowship Nov. 2014/Sept. 2015, ref: ICIQ-SCP, Spanish Ministry of Science and Innovation.
- 2014: Master best mark promotion award 2014.
- 2013: Bachelor best mark promotion award 2013.
- 2013: Collaboration Fellowship Spanish Ministry MECD (most competitive Research fellowship at degree level) 2013.
- 2012: Fellowship *Xavier Gironès* Univ. Girona 2012.
- 2009: Fellowship “Beca Caixa Manresa” to cover the first year of my Chemistry degree for being top class student in the exams to access university (PAU).
- 2009: Award “Félix Garcia Castañer” from the Rotary Club Costa Brava (remarkable scientific record and research project). Stay in Darmstadt visiting the “Technische Universität Darmstadt” and ESOC, 2009.

## 6. Internationalization

In her 9 years of career (since the beginning of her master's) Dr. Casadevall has worked in 8 internationally recognized institutions (University of Girona, ICIQ, URV, ASU, MPI-CEC, KTH, University of Groningen, University of Cambridge) in 6 different countries (Spain, Sweden, US, Netherlands, Germany, UK), and performed short stays in 3 different synchrotrons in Spain and UK.

- Oct. 2021: ALBA synchrotron in Spain as part of an awarded beamtime proposal as PI (ref: 2021025005) in collaboration with Dr. Vlad Martin-Diaconescu (ALBA synchrotron scientist).
- Sept. 2019-Oct. 2022: Postdoc (BBSRC and MSCA IF) at the Reisner Lab at the **University of Cambridge**.
- Nov. to Dec. 2018: short PhD stay at **Max Planck Institute for Chemical Energy Conversion** (MPI-CEC) in Germany, collaboration with Prof. S. DeBeer and Dr. O. Rüdiger. Activities: EPR spectroelectrochemistry, Raman and X-ray studies to characterize high-valent water oxidation intermediates. – *Manuscript under revision*.
- Jul. 2018: stay at the **Faculty of Science and Engineering, Molecular Inorganic Chemistry — Stratingh Institute for Chemistry** at the University of Groningen in The Netherlands, collaboration with Prof. W. R. Browne (2 short stays of about 9 days each). Activities: Raman studies of in-situ and isolated intermediates in water oxidation. – 1<sup>st</sup> author manuscript (*Nat. Chem.* 2021, 13, 800).
- Apr. to Jul. 2018: long PhD stay at **Arizona State University — School of Molecular Sciences** in the United States, collaboration with the group of Prof. G. Ghirlanda. Activities: Effect of tuning the second coordination sphere of Co complexes in water reduction by the development of Co-streptavidin artificial metalloenzyme for water reduction. And development of a semiartificial Co cytochrome metalloenzyme for photoelectrocatalyzed water splitting. – 1 Manuscript as co-first author (*ACS Catal.* 2019, 9 (7), 5837), and 1 manuscript as first and corresponding author (*Catalysts* 2021, 11(5), 626; <https://doi.org/10.3390/catal11050626>) published.
- During 2015-2017: 4 Synchrotron trips: **SOLEIL – LUCIA** beamline (France), **DIAMOND** (UK), 2x **SOLEIL-SAMBA** beamline (France). Activities: X-ray characterization of Ru and Fe intermediates in water oxidation, and low-valent Co-intermediates involved in water and CO<sub>2</sub> reduction. 1<sup>st</sup> author manuscript (*Nat. Chem.* 2021, 13, 800) and coauthored manuscript (*J. Am. Chem. Soc.* 2020, 142 (1), 120).
- Sept. 2015: short PhD stay at **KTH Royal Institute of Technology** in Sweden, at the group of Prof. M. Ahlquist as an awardee of the COST travel PhD grant. Activities: computational studies → DFT and CASSCF calculations of EPR of Co intermediates in light-driven water reduction.

## 7. Leadership

### Projects

- PI in the awarded Spanish National Research Grant 2022, ref:PID2022-142975OA-I00, BiSoRAP “*Microfotoreactores polimericos bioinspirados funcionalizados con catalizadores para fotosintesis artificial*”, URV (2023-2026), 125.000,00 €.

- Co-PI in the awarded FEDER AGAUR 2021 PROD 00043 “Fotoreactor de flow intel·ligent per industrialitzar reaccions fotoquímiques” (Smart Flow Photoreactor to Industrialize Chemical Reactions), from “Generalitat de Catalunya”, ICIQ, 2022-2024. 99.961,00 €, PI Scientific Entrepreneur.
- PI in the awarded Ramón y Cajal project call 2022. Ref: RYC2021-030935-I. URV, 01/01/2023 – 31/12/2027, 236.350,00 €.
- PI in the awarded project 117489. Semiartificial Soft Material LEGOs for Solar Fuels and Chemicals (LEGO4Chem). La Caixa Junior Leader Incoming Program, call 2022, ref: 117489, ICIQ, 01/10/2022 – 31/09/2025, 305.100,00 €.
- PI in the awarded project: 2021025005 - Characterization of low valent Ni(II) and Ni(I) and high valent Ni(III) species involved in catalytic C-O and C-N bond formation by a heterogeneous Ni-single site on porous carbon nitride. ALBA synchrotron, call 2021, University of Cambridge 18/10/2021-21/10/2021. 60.000,00 €.
- Co-PI in the successful outreach project “Joves I Ciència 2022 – project Artificial Photosynthesis”.
- PI in the PR00P2\_208614 PRIMA Grant. Semiartificial Soft Material LEGOs for Solar Fuels and Chemicals (LEGO4Chem). Swiss National Science Foundation (SNSF), call 2022. Submitted 01/11/2021 (selected for Stage 2 – interview, not awarded). 1.331.548,06 €.

### Student supervision

- **Current PhD thesis director** of Ms. Laura Velasco Garcia (Oct. 2023 – Sept. 2027) and Mr. Edelman Espinoza Suarez (Oct. 2023 – Sept. 2027) at URV/ICIQ.
- **Current Master thesis director** of Mr. Akhmet Bekaliyev (Oct. 2023 – Sept. 2024), and **previous Master thesis director** of Ms. Laura Velasco Garcia (Oct. 2022 – Sept. 2023).
- Previous student supervision: 5 PhD students (D. Pascual (ICIQ), D. Kim, A. Vijeta, A. Lage, V. Badiani (Cambridge)), 4 Master students (D. S. Zijlstra; L. Montiel, I. Rosa, A. Albert Flores) and 2 undergraduate students (A. Gotaire, I. Rosa).

### Papers as corresponding author

- 3 papers as corresponding author without my PhD nor my Postdoc Advisors (EAES, ISSN: 2578-0336, 2020 and Catalysts 2021, 11(5), 626; <https://doi.org/10.3390/catal11050626>).

### Commissions of Trust, Reviewer and Editorial Duties

- Appointed as Research Associate at Peterhouse College (Cambridge) since January 2020.
- Review Editor on the Editorial Board of Solar Fuels (specialty section of Frontiers in Fuels, since 2022).
- Review Editor on the Editorial Board of Green and Sustainable Chemistry (specialty section of Frontiers in Chemistry, since 2022).
- Reviewer for a Postdoctoral Fellowship from a German Agency.
- Topic editor of Catalysts journal from MDPI (since April 2021).
- Project manager of the UK Solar Fuels Network (<https://www.solarfuelsnetwork.com/>) (Sept. 2019/Dec. 2020)
- Member of Scientific Evaluation Panel at AQU (University Quality Agency, 2013-2018) evaluating University program.
- Member of Scientific Evaluation Panel at ASIIN quality agency for the assessment of EUROMASTER label (June 2018).
- PhD viva examiner: Mr. Ignacio Rosa Pardo (21/11/23 University of Valencia, Spain); Dr. Eleni Georgiou (27/06/2023 ICIQ, Spain); Dr. Klaudia Michaliszyn (22/04/22 ICIQ, Spain); External examiner Dr. Geyla C. Dubed (14/11/22, ICIQ, Spain).
- Referee in > 15 peer-reviewed articles, including Nat. Cat., JACS, Chem. Sci., ACS Catal., among others.

### 8. Professional Membership in Scientific Societies

- Catalan Chemical Society (SCQ), Spain, since 2023.
- Research Associate at Peterhouse College, Cambridge, since January 2020.
- UK Solar Fuels Network, since 2019.
- RSEQ (Spanish Royal Society of Chemistry), Spain, since 2014.
- JIQ (Young Chemical Researchers), Spain, since 2014.
- GEQO (Organometallic Chemistry Division) from RSEQ, Spain, since 2014.
- GEEN (Energy and Sustainability) from RSEQ, Spain, since 2022.
- GEP (Polymers) from RSEQ, Spain, since 2022.
- IUPAC member since 2022.

### 10. Publications (\*corresponding author, †equal contribution, #1<sup>st</sup> author is a supervised student)

#### From PhD at ICIQ (Nov 2014 to July 2019) and short postdoc (July 2019 to September 2019):

1. A. Moneo-Corcuera, D. Nieto-Castro, J. Cirera, V. Gómez, J. Sanjosé-Orduna, **C. Casadevall**, G. Molnár, A. Bousseksou, T. Parella, J. María Martínez-Agudo, J. Lloret-Fillol, M. Hevia Pérez-Temprano, E. Ruiz, J. R. Galán-Mascarós, “Synthesis and characterization of highly diluted polyanionic iron (II) spin crossover systems”; *STAR Protocols*, 2023, 4, 102394, <https://doi.org/10.1016/j.xpro.2023.102394>

2. A. Moneo-Corcuera, D. Nieto-Castro, J. Cirera, V. Gómez, J. Sanjosé-Orduna, **C. Casadevall**, G. Molnár, A. Bousseksou, T. Parella, J. María Martínez-Agudo, J. Lloret-Fillol, M. Hevia Pérez-Temprano, E. Ruiz, J. R. Galán-Mascarós “Molecular magnetic memory near room temperature in an iron polyanionic complex”; *Chem*, 2023, 9, 2, 377-393, <https://doi.org/10.1016/j.chempr.2022.09.025>.
3. **C. Casadevall**<sup>‡</sup>, J. Aragón<sup>‡</sup>, S. Cañellas, M. A. Pericàs, J. Lloret-Fillol, X. Caldentey, “Development of Advanced High Throughput Experimentation Platforms for Photocatalytic Reactions”. The Power of High-Throughput Experimentation: General Topics and Enabling Technologies for Synthesis and Catalysis (Volume 1), Chapter 9, 145-165, *ACS Symposium Series*, 2022, 1419, doi: 10.1021/bk-2022-1419.ch009.
4. **C. Casadevall**, D. Pascual, J. Aragón, A. Call, A. Casitas, I. Casademont-Reig, J. Lloret-Fillol, “Light-Driven Reduction of Aromatic Olefins in Aqueous Media Catalysed by Aminopyridine Cobalt Complexes”; *Chem. Sci.* 2022,13, 4270-4282, <https://doi.org/10.1039/D1SC06608K>, advance article. Front Cover.
5. N. Levin, **C. Casadevall**, G. E. Cutsail III, T. Weyhermüller, J. Lloret-Fillol, S. DeBeer, O. Rüdiger, “XAS and EPR in situ observation of Ru(V) oxo intermediate in a Ru water oxidation complex”; *ChemElectroChem*, 2021, 9, e20210127, <https://doi.org/10.1002/celec.202101271>. Front Cover.
6. **C. Casadevall**, V. Martin-Diaconescu, W.R. Browne, S. Fernández, F. Franco, N. Cabello, J. Benet-Buchholz, B. Lassalle-Kaiser, J. Lloret-Fillol, “Isolation of a side-on ruthenium(IV)-peroxo intermediate after the rate determining step in the water oxidation reaction”; *Nat. Chem.* 2021, 13, 800-804, <https://doi.org/10.1038/s41557-021-00702-5>, Highlighted by C.C. Cody and G. W. Brudvig in *Joule* 5, 1921–1933, August 18, 2021; *Nature Portfolio Chemistry Community*, May 2021; and in different news and blogs such as: Chemeurepe.com; Azomaterials; Sciencenewsnet.in; Infosurhoy; Bioengineer; Scienmag; SciTechDaily; Phys.org.
7. **C. Casadevall**<sup>\*</sup>, H. Zhang, S. Chen, D. J. Sommer, D. Seo, G. Ghirlanda, “Photoelectrochemical Water Splitting with Cobalt Cytochrome c integrated-ATO Photoanode”; *Catalysts*, 2021, 11(5), 626-637. <https://doi.org/10.3390/catal11050626>
8. S. d’Agostini, K. Kotttrup, **C. Casadevall**, I. Gamba, M. Costas, J. Lloret-Fillol, D. Hatterscheid, “Electrocatalytic water oxidation with  $\alpha$ -[Fe(mcp)(OTf)<sub>2</sub>] and analogues”; *ACS Catal.*, 2021, 11, 5, 2583–2595. <https://doi.org/10.1021/acscatal.0c05439>
9. I. Rosa-Pardo, **C. Casadevall**, L. Schmidt, M. Claros, R. E. Galian, J. Lloret-Fillol, J. Pérez-Prieto, “The Synergy between the CsPbBr<sub>3</sub> Nanoparticle Surface and the Organic Ligand Becomes Manifest in a Demanding Carbon-Carbon Coupling Reaction”; *Chem. Commun.* 2020, 56, 5026-5029. <https://doi.org/10.1039/D0CC01339K>
10. S. Fernández, F. Franco, **C. Casadevall**, V. Martin-Diaconescu, J.M. Luis, J. Lloret-Fillol; “A Unified Electro- and Photocatalytic CO<sub>2</sub> to CO Reduction Mechanism with Aminopyridine Cobalt Complexes.”; *J. Am. Chem. Soc.* 2020, 142 (1), 120-133. <https://doi.org/10.1021/jacs.9b06633>
11. **C. Casadevall**<sup>\*</sup>, “Current Opinion In Artificial Photosynthesis with Molecular Catalysts”, *EAES*, ISSN: 2578-0336, 2020. 10.31031/EAES.2020.07.000651
12. **C. Casadevall**, A. Bucci, M. Costas, J. Lloret-Fillol; “Water Oxidation Catalysis with Well-defined Molecular Iron Complexes”; *Adv. Inorg. Chem.* 74, 2019, 151-196. <https://doi.org/10.1016/bs.adioch.2019.03.004>
13. A. Call<sup>‡</sup>, **C. Casadevall**<sup>‡</sup>, A. Romero-Rivera, D. J. Sommer, S. Osuna, G. Ghirlanda, and J. Lloret-Fillol, “Improved Activity and Stability of an Electro- and Photocatalytic Water Reduction Cobalt Catalyst by Supramolecular Confinement in Streptavidin”; *ACS Catal.* 2019, 9 (7), 5837-5846. <https://doi.org/10.1021/acscatal.8b04981>
14. Z. Codolà, I. Gamba, F. Acuña-Parés, **C. Casadevall**, M. Clémancey, J-M. Latour, J. M. Luis, M. Costas, J. Lloret-Fillol; “Design of Iron Coordination Complexes as Highly Active Homogenous Water Oxidation Catalysts by Deuteration of Oxidation Sensitive Sites”; *J. Am. Chem. Soc.*, 2019, 141 (1), 323-333. <https://doi.org/10.1021/jacs.8b10211>
15. A. Call<sup>‡</sup>, **C. Casadevall**<sup>‡</sup>, F. Acuña-Parés, A. Casitas, J. Lloret-Fillol; “Dual cobalt-copper light-driven catalytic reduction of aldehydes and aromatic ketones in aqueous media”; *Chem. Sci.* 2017, 8 (7), 4739- 4749.

<https://doi.org/10.1039/C7SC01276D> Front cover, Highlighted in Chemistry World and Chemistry Views and This article is part of the themed collection: Most downloaded articles of 2017: Energy and Catalysis.

16. C. Casadevall, A. Call, Z. Codolà, F. Acuña-Parés, J. Lloret-Fillol; “Catalizadores para la conversión de la energía solar en enlaces químicos”; *An. Quim.* 2016, 112 (3), 133-141.

17. C. Casadevall, Z. Codola, M. Costas, J. Lloret-Fillol, “Spectroscopic, Electrochemical and Computational Characterization of Ru Species Involved in Catalytic Water Oxidation: Evidence for a [Ru<sup>V</sup>(O)(Py<sub>2</sub>Metacn)] Intermediate”, *Chem. Eur. J.* 2016, 22 (29), 10111- 10126. <https://doi.org/10.1002/chem.201600584>

**From Postdoc at University of Cambridge (Sept. 2019 to actual):**

18. C. Casadevall, A. Lage, M. Mu, H. F. Greer, D. Antón-García, J. N. Butt, L. J. C. Jeuken, G. W. Watson, M. García-Melchor, E. Reisner, “Size-dependent activity of carbon dots for photocatalytic H<sub>2</sub> generation in combination with a molecular Ni cocatalyst”, *Nanoscale* 2023, advance articles, *accepted, in press.*

19. H. Zhang<sup>‡</sup>, C. Casadevall<sup>‡</sup>, J. H. van Wonderen, L. Su, J. N. Butt, E. Reisner, L. Jeuken, “Rational Design of Covalent Multiheme Cytochrome-Graphitic Carbon Dot Biohybrids for Photo-induced Electron Transfer”, *Adv. Funct. Mat.* 2023, 2302204, *Accepted, in press.*

20. T. Lawson, A. Gentleman, A. Lage, C. Casadevall, J. Xiao, T. Petit, M. Frosz, E. Reisner, T. Euser, “Low-Volume Reaction Monitoring of Carbon Dot Light Absorbers in Optofluidic Microreactors”, *ACS Catal.* 2023, 13, 9090-9101, <https://doi.org/10.1021/acscatal.3c02212>

21. D. A. Garcia-Osorio, T. P. Shalvey, L. Banerji, K. Saeeda, G. Neria, L. J. Phillips, O. S. Huttera, C. Casadevall, D. Antón-García, E. Reisner, J. D Majora, A. J Cowan, “Hybrid photocathode based on Ni molecular catalyst and Sb<sub>2</sub>Se<sub>3</sub> for solar H<sub>2</sub> production”, *Chem Comm.* 2023, 59, 944-947. Doi:10.1039/d2cc04810h.

22. L. Gutiérrez, V. Martin-Diaconescu, C. Casadevall, F. Oropeza, V. A. de la Peña O’Shea, J. Meng, M. A. Ortuño, J. Lloret-Fillol; “Low Oxidation State Cobalt Center Stabilized by a Covalent Organic Framework to Promote Hydroboration of Olefins”, *ACS Catal.* 2023, 13, 3044-3054. <https://doi.org/10.1021/acscatal.2c05442>.

23. S. EH Piper, C. Casadevall, E. Reisner, T. A. Clarke, L. JC Jeuken, A. J Gates, J. N. Butt, “Photocatalytic Removal of the Greenhouse Gas Nitrous Oxide by Liposomal Microreactors”, *Angew. Chem. Int. Ed.*, 2022, 61, e202210572, [doi.org/10.1002/anie.202210572](https://doi.org/10.1002/anie.202210572), hot paper.

24. V. M. Badiani, C. Casadevall<sup>#</sup>, M. Miller, A. R. Oliveira, I. A. C. Pereira, E. Reisner, “Engineering Electro- and Photocatalytic Carbon Materials for CO<sub>2</sub> Reduction by Formate Dehydrogenase”, *J. Am. Chem. Soc.* 2022, 144, 31, 14207-14216, <https://doi.org/10.1021/jacs.2c04529>.

25. C. Casadevall\*, “Heterogenisation of molecular Water Oxidation Catalysts in electrodes for (Photo)electrochemical Water Oxidation”; *Water*, 2022, 14(3), 371; <https://doi.org/10.3390/w14030371>.

26. Vijeta, C. Casadevall<sup>#</sup>, E. Reisner, “Integrated Carbon Nitride-Nickel Heterogeneous Material as Photocatalyst for Amination of Aryl halides using Sodium Azide”; *Angew. Chem. Int. Ed.*, 2022, Accepted Articles. <https://doi.org/10.1002/anie.202203176>. Highlighted as VIP.

27. T. Li, A. Vijeta, C. Casadevall, A. Gentleman, T. Euser, E. Reisner, “Bridging Plastic Recycling and Organic Catalysis: Photocatalytic Deconstruction of Polystyrene via C-H Oxidation Pathway”, *ACS Catal.* 2022, 12, 14, 8155-8163, <https://doi.org/10.1021/acscatal.2c02292>.

28. Pannwitz, D. M. Klein, S. Rodriguez-Jimenez, C. Casadevall, H. Song, E. Reisner, L. Hammarström, S. Bonnet, “Roadmap for photoredox catalysis at the water interface of lipid membranes”; *Chem. Soc. Rev.* 2021, 50, 4833-4855 Advanced Article – Tutorial Review, [doi.org/10.1039/D0CS00737D](https://doi.org/10.1039/D0CS00737D).

29. Vijeta, C. Casadevall<sup>#</sup>, S. Roy, E. Reisner, “Visible-Light Promoted C–O Bond Formation with an Integrated Carbon Nitride–Nickel Heterogeneous Photocatalyst”; *Angew. Chem. Int. Ed.*, 2021, 60, 8494–8499. <https://doi.org/10.1002/anie.202016511>

30. S. E. H. Piper, M. J. Edwards, J. H van Wonderen, C. Casadevall, A. Martel, L. J. C. Jeuken, E. Reisner, T. A. Clarke, J. N. Butt,” Bespoke Biomolecular Wires for Transmembrane Electron Transfer: Spontaneous Assembly

of a Functionalized Multiheme Electron Conduit”; *Front. Microbiol.*, 2021, 12:714508, doi.org/10.3389/fmicb.2021.714508.

31. Z. Wen, T. Wan, A. Vijeta, C. Casadevall, L. Buglioni, E. Reisner, T. Noël, “Photocatalytic C–H Azolation of Arenes using Heterogeneous Carbon Nitride in batch and flow”; *ChemSusChem*, 2021, 14, 5265. <https://doi.org/10.1002/cssc.202101767>.

## 11. Technology transfer

### Patents:

1. J. Lloret-Fillol, C. Casadevall, J. León, A. Call, A. Casitas, J. J. Pla, J. P. Hernández, X. F. Caldentey: EP3612300 - PHOTOREACTOR. Submitted as: European Patent. Fundació privada Institut Català d’Investigació Química and Institució Catalana de Recerca I Estudis Avançats (Application Number: 18727800.7, Priority Number: EP20170382313, filling date 30.05.2018, priority date 31.05.2017, granted date 09/2020, Original published format: EP 17382313). Licensed and exploited patent by [Trellum technologies](https://register.epo.org/application?number=EP18727800&tab=main) spin off, currently prototyping and doing the industrialization of the photoreactor. <https://register.epo.org/application?number=EP18727800&tab=main>
2. J. Lloret-Fillol, A. Call, C. Casadevall, A. Casitas. WO2018211154 - PHOTOCATALYTIC REDUCTION PROCESS AND CATALYTIC COMPOSITION USED IN THE PROCESS. Submitted as: PCT. Fundació privada Institut Català d’Investigació Química and Institució Catalana de Recerca I Estudis Avançats (Application Number: 17729906.2, PCT/ES2017/070314, filling date 16.05.2017, granted date 22.11.2018). <https://register.epo.org/application?number=EP17729906>

## 12. Conferences/invited talks

### 12 Invited talks:

- 1) **MPI-CEC seminar program 20/11/2018** (Germany) “Isolation of a missing link in the water oxidation reaction” (45 min). Invited by Prof. Serena DeBeer and Dr. Olaf Rüdiger.
- 2) **Gordon Research Symposium Solar Fuels 07/05/2022** (Italy) “Unifying the principles of electro- and photocatalytic CO<sub>2</sub> reduction with formate dehydrogenase interfaced with carbon nanotubes and carbon dots” (15 min). Invited by Dr. Shannon Bonke and Dr. Ana Maria Beiler.
- 3) **University Complutense de Madrid**, Department of Chemistry seminar program 17/11/2022 (Spain) “Carbon-based materials for solar-driven catalysis” (45 min). Invited by Dr. Carmen Martín Gandul.
- 4) **Photocatalysis Workshop, Lorenz Conferences**, 27-30/03/2023, Leiden (Netherlands), organized by the Lorentz Center, Dr. Sojia Pullen, Dr. Line Naesborg and Dr. Sebastian Beil. Invited short talk.
- 5) **PhD Day University of Valladolid 13/04/2023** (Spain) “Carbon-based materials for solar-driven catalysis”. Invited by Dr. Álvaro García and Prof. Juan Casares (organizing committee).
- 6) **NanoSpain Conference 25-28/04/2023** (Spain) “Carbon-based materials for solar-driven catalysis”. Invited by Dr. Antonio Correia and Dr. Jose Luis Roldan.
- 7) **II Symposium in Molecular Chemistry and Catalysis** at the Institute of Chemical Synthesis and Homogeneous Catalysis (iSQCH), CSIC and University of Zaragoza 16/06/2023 (Spain) “From molecular systems to hybrid materials for solar-driven catalysis” (Plenary Lecture). Invited by Prof. Pablo Sanz de Miguel.
- 8) **Kroese Duijsters symposium, University of Leiden 19-20/06/2023** (Netherlands) “From molecular systems to hybrid materials for solar-driven catalysis”. Invited by Prof. Lars Jeuken, Prof. Marc Koper and Prof. Dennis Hetterscheid (University of Leiden).
- 9) **VI ICIQ PhD Day 2023**, Tarragona (Spain), organized by ICIQ and URV. “From molecular systems to hybrid materials for solar-driven catalysis”.
- 10) **XIX Young Researchers Symposium RSEQ-Sigma Aldrich 2023**, 13-16/11/2023, Murcia (Spain), organized by the Spanish Royal Society of Chemistry (RSEQ) and the University of Murcia. Invited talk as a 2023 RSEQ young investigator Prize winner. “From molecular systems to hybrid materials for solar-driven catalysis”.

**11) 13<sup>th</sup> Congress of the Young Researchers of the Catalan Countries 2024**, Tarragona (Spain), organized by the Catalan Chemical Society and the University Rovira i Virgili. Invited talk as Plenary Speaker.

**12) 4<sup>th</sup> Frontiers In Photochemistry Conference**, 10-13/07/2023, Lisbon (Portugal), organized by Fusion Conferences. Invited talk as Invited Speaker.

### **13 Oral presentations in national and international conferences:**

- 1) Symposium in Organometallic and inorganic Chemistry from the Catalan Chemical Society (RQIO, SCQ) 2023**, Barcelona (Spain), organized by the SCQ, University Rovira i Virgili (URV) and the University of Barcelona (UB). Talk: **Carla Casadevall**, Vivek M. Badiani, Ava Lage, Max Garcia-Melchor, Erwin Reisner. "Carbon-based materials for solar-driven catalysis".
- 2) XVIII Young Researchers Symposium RSEQ-Sigma Aldrich 2022**, Seville (Spain), organized by the Spanish Royal Society of Chemistry (RSEQ), the University of Seville and CIC Cartuja. Talk: **Carla Casadevall**, Vivek M. Badiani, Ava Lage, Max Garcia-Melchor, Erwin Reisner. "Carbon dots for photocatalytic applications: from water and CO<sub>2</sub> reduction to organic methodology".
- 3) Post ICCC (International Conference of Coordination Chemistry) 2018**, Fukuoka (Japan), organized by the University of Kyushu. Talk: **Carla Casadevall**; Vlad Martin-Diaconescu; Wesley Browne; Federico Franco; Noemí Cabello; Jordi Benet Buchholz; Benedikt Lasalle Kaiser; Julio Lloret Fillol. "Isolation and Characterization of an elusive  $\eta^2$ -[Ru(IV)-OO]<sup>2+</sup> intermediate after the O-O bond formation in Ru catalyzed WO: a missing link".
- 4) 43rd ICCC (International Conference of Coordination Chemistry) 2018**, Sendai (Japan), organized by the University of Kyushu. Talk: **Carla Casadevall**; Vlad Martin-Diaconescu; Wesley Browne; Federico Franco; Noemí Cabello; Jordi Benet Buchholz; Benedikt Lasalle Kaiser; Julio Lloret Fillol. "Isolation and Characterization of an elusive  $\eta^2$ -[Ru(IV)-OO]<sup>2+</sup> intermediate after the O-O bond formation in Ru catalyzed WO: a missing link".
- 5) Girona Seminar 2018**, Girona (Spain), organized by the IQCC (Institute of Computational Chemistry and Catalysis) University of Girona. Talk: **Carla Casadevall**; Vlad Martin-Diaconescu; Wesley Browne; Federico Franco; Noemí Cabello; Jordi Benet Buchholz; Benedikt Lasalle Kaiser; Julio Lloret Fillol. "Isolation and Characterization of an elusive  $\eta^2$ -[Ru(IV)-OO]<sup>2+</sup> intermediate after the O-O bond formation in Ru catalyzed WO: a missing link".
- 6) H<sub>2</sub>BioCatO<sub>2</sub> RED meeting 2017 (National Conference form a National Network working on Artificial Photosynthesis)**, Castellón (Spain), organized by the RED H<sub>2</sub>BioCatO<sub>2</sub> and University of Cádiz. Talk: **Carla Casadevall**; Vlad Martin-Diaconescu; Wesley Browne; Federico Franco; Noemí Cabello; Jordi Benet Buchholz; Benedikt Lasalle Kaiser; Julio Lloret Fillol. "Isolation and Characterization of an elusive  $\eta^2$ -[Ru(IV)-OO]<sup>2+</sup> intermediate after the O-O bond formation in Ru catalyzed WO: a missing link".
- 7) ICIQ PhD day 2017**, Tarragona (Spain), organized by ICIQ. Talk: **Carla Casadevall**, Arnau Call; Ferran Acuña Parés; Alicia Casitas, Julio Lloret Fillol. "Dual cobalt-copper light-driven catalytic reduction of aldehydes and aromatic ketones and olefins in aqueous media".
- 8) BIST PhD day 2017**, Tarragona (Spain), organized by ICIQ. Talk: **Carla Casadevall**, Julio Lloret Fillol. "Solar Fuels and Artificial Photosynthesis".
- 9) CARISMA meeting 2017**, Lisbon (Portugal), organized by the COST CARISMA ACTION, University nova de Lisboa and Institute of Chemical and Biological Technology Antonio Xavier. Talk 1: **Carla Casadevall**; Marten Ahlquist; Julio Lloret Fillol. "Computational Characterization of the Co Intermediates involved in Co-catalyzed water oxidation and water reduction reactions".
- 10) CARISMA meeting 2017**, Lisbon (Portugal), organized by the COST CARISMA ACTION, University nova de Lisboa and Institute of Chemical and Biological Technology Antonio Xavier. Talk 2: **Carla Casadevall**; Zoel Codolà; Ilaria Gamba; Ferran Acuña Parés; Josep Maria Luis Luis; Julio Lloret Fillol; Miquel Costas. "Determination of the molecular nature of Fe-WOC based on aminopyridyl ligands".
- 11) XII Young Researchers Symposium RSEQ-Sigma Aldrich 2015**, Barcelona (Spain), organized by the Spanish Royal Society of Chemistry (RSEQ). Talk: **Carla Casadevall**; Alicia Casitas; Ferran Acuña Parés; Arnau Call; Julio Lloret Fillol. "Light-driven cobalt catalysed reduction of olefins using water as a source of protons".

- 12) Summer School in molecular catalysts 2015 (Heidelberg university) in the Heidelberg Centre of Latin America in Santiago de Chile (Chile), organized by the University of Heidelberg. Talk: **Carla Casadevall**; Julio Lloret Fillol. "Light-driven metal catalyzed organic transformations".
- 13) XI Young Researchers Symposium RSEQ-Sigma Aldrich 2014, Bilbao (Spain), organized by the Spanish Royal Society of Chemistry (RSEQ). Talk: **Carla Casadevall**; Zoel Codolà; Miquel Costas; Julio Lloret Fillol. "Unravelling the mechanism of water oxidation catalysed by novel tacn-based ruthenium complexes".

#### 16 poster presentations in national and international conferences:

- 1) Lorentz Center invited workshop - *Photocatalysis – challenges and future perspectives* 2023, Leiden (Netherlands), organized by Dr. Sonja Pullen (University of Amsterdam), Dr. Sebastian Beil (Stratingh Institute for Chemistry, University of Groningen), Dr. Line Næsberg (WWU Münster). Poster: **Carla Casadevall**, Vivek V. Badiani, Ava Lage, Sam J. Cobb, Melanie Miller, Ana M Coito, Ines A. C. Pereira, Erwin Reisner. "Carbon dots for solar fuels: CD size dependent activity in HER and understanding the orientation of FDH interfaced with CNTs and CDs for electro- and photocatalytic CO<sub>2</sub> reduction".
- 2) Gordon Research Conference (GRC): Solar Fuels 2022, Tuscany (Italy), organized by the GRC. Poster: **Carla Casadevall**, Vivek V. Badiani, Ava Lage, Sam J. Cobb, Melanie Miller, Ana M Coito, Ines A. C. Pereira, Erwin Reisner. "Carbon dots for solar fuels: CD size dependent activity in HER and understanding the orientation of FDH interfaced with CNTs and CDs for electro- and photocatalytic CO<sub>2</sub> reduction".
- 3) SuperSolar-SFN workshop 2019, London (UK), organized by SuperSolar and the Solar Fuels Network (UK). Poster 1: **Carla Casadevall**; Annika Eisenschmidt, Erwin Reisner. "Solar Fuels Network".
- 4) SuperSolar-SFN workshop 2019, London (UK), organized by SuperSolar and the Solar Fuels Network (UK). Poster 2: **Carla Casadevall**; Vlad Martin-Diaconescu; Wesley Browne; Federico Franco; Noemí Cabello; Jordi Benet Buchholz; Benedikt Lasalle Kaiser; Julio Lloret Fillol. "Isolation and Characterization of an elusive  $\eta^2$ -[Ru(IV)-OO]<sup>2+</sup> intermediate after the O-O bond formation in Ru catalyzed WO: a missing link".
- 5) Faraday Discussions 2019, Cambridge (UK), organized by the University of Cambridge. Poster: **Carla Casadevall**; Vlad Martin-Diaconescu; Wesley Browne; Federico Franco; Noemí Cabello; Jordi Benet Buchholz; Benedikt Lasalle Kaiser; Julio Lloret Fillol. "Isolation and Characterization of an elusive  $\eta^2$ -[Ru(IV)-OO]<sup>2+</sup> intermediate after the O-O bond formation in Ru catalyzed WO: a missing link".
- 6) TrapCat2 (Transpyrenean meeting in Catalysis) 2018, Tarragona (Spain), organized by the University Rovira i Virgili (URV). Poster: **Carla Casadevall**; Vlad Martin-Diaconescu; Wesley Browne; Federico Franco; Noemí Cabello; Jordi Benet Buchholz; Benedikt Lasalle Kaiser; Julio Lloret Fillol. "Isolation and Characterization of an elusive  $\eta^2$ -[Ru(IV)-OO]<sup>2+</sup> intermediate after the O-O bond formation in Ru catalyzed WO: a missing link".
- 7) ICHAT (International Congress for Hydrogen Atom Transfer) 2017, Frascati-Rome (Spain), organized by University of Roma "Tor Vergata" and "La Sapienza" and University of British Columbia. Poster: **Carla Casadevall**; Arnau Call; Ferran Acuña Parés; Alicia Casitas, Julio Lloret Fillol. "Dual cobalt-copper light-driven catalytic reduction of aldehydes and aromatic ketones and olefins in aqueous media".
- 8) Girona Seminar 2016: predictive catalysis, Girona (Spain), organized by the University of Girona, IQCC (Institute of Computational Chemistry and Catalysis). Poster: **Carla Casadevall**; Alicia Casitas Montero; Arnau Call Quintana; Julio Lloret Fillol. "Light-driven cobalt catalysed reduction of olefins using water as a source of protons".
- 9) GEQO (Organometallic Chemistry Congress)-RSEQ (Spanish Royal Society of Chemistry) 2016, Girona (Spain), organized by the University of Girona, IQCC (Institute of Computational Chemistry and Catalysis) and RSEQ-GEQO. Poster: **Carla Casadevall**; Alicia Casitas; Julio Lloret Fillol. "Light-driven Cobalt catalysed reduction of olefins using water/amines as a source of hydrogen".
- 10) Spain-Japan Joint Symposium on Theoretical and Computational Chemistry of Complex systems 2015, Tarragona (Spain), organized by ICIQ (Institute of Chemical Research of Catalonia) and Fukui Institute for Fundamental Chemistry. Poster: **Carla Casadevall**; Zoel Codolà; Miquel Costas; Julio Lloret Fillol. "Unravelling the mechanism of water oxidation catalyzed by novel tacn-based ruthenium complexes".
- 11) Pacificchem: the international chemical congress of pacific basin societies 2015, Honolulu-Hawaii (USA), organized by the American Chemical Society, chemical Society of Japan and Canadian Society for Chemistry. Poster: **Carla**



**Casadevall**; Zoel Codolà; Miquel Costas; Julio Lloret Fillol. “Unravelling the mechanism of water oxidation catalyzed by novel tacn-based ruthenium complexes”.

- 12) OMCOS 18 (Organometallic Chemistry Directed Towards Organic Synthesis), Sitges (Spain), organized by the Spanish Royal Society of Chemistry (RSEQ). Poster: **Carla Casadevall**; Zoel Codolà; Miquel Costas; Julio Lloret Fillol. “Unravelling the mechanism of water oxidation catalyzed by novel tacn-based ruthenium complexes”.
- 13) Summer School in Molecular Catalysts 2015 (Heidelberg university) in the Heidelberg Centre of Latin America in Santiago de Chile (Chile), organized by the University of Heidelberg. Poster: **Carla Casadevall**; Julio Lloret Fillol. “Light-driven metal catalyzed organic transformations”.
- 14) Summer School Theory and Practice in Spectroscopy (COST) 2015, Groningen (Netherlands), organized by COST action and University of Groningen. Poster: **Carla Casadevall**; Zoel Codolà; Miquel Costas; Julio Lloret Fillol. “Unravelling the mechanism of water oxidation catalyzed by novel tacn-based ruthenium complexes”.
- 15) Summer School in Organic Synthesis A. Corbella (CARISMA-COST) 2015, Italy (Spain), Organized by COST-CARISMA. Poster: **Carla Casadevall**; Zoel Codolà; Miquel Costas; Julio Lloret Fillol. “Unravelling the mechanism of water oxidation catalyzed by novel tacn-based ruthenium complexes”.
- 16) CARISMA-COST meeting 2015, Tarragona (Spain), organized by COST-CARISMA and ICIQ. Poster: **Carla Casadevall**; Zoel Codolà; Miquel Costas; Julio Lloret Fillol. “Unravelling the mechanism of water oxidation catalyzed by novel tacn-based ruthenium complexes”.

#### 8 Conference/seminar organization:

- 1) Chair of the ICIQ seminar program sponsored by the BASF during 2023.
- 2) Chair of the ICIQ symposium “Frontiers in Renewable Fuels and Chemicals” 7 March 2023
- 3) Co-Chair of the NanoGe MATSUS meeting 2023 – Symposium e-FuelSyn, March 8-10 Valencia, Spain.
- 4) Organizing committee of the 8<sup>th</sup> SFN Symposium 2020 (online), organized by the Solar Fuels Network and the University of Liverpool (UK).
- 5) Organizing committee of the TrapCat2 (Transpyrenean meeting in Catalysis) 2018, Tarragona (Spain), organized by the University Rovira i Virgili (URV).
- 6) Organizing committee of the XII Young Researchers Symposium RSEQ-Sigma Aldrich 2015, Barcelona (Spain), organized by the Spanish Royal Society of Chemistry (RSEQ).
- 7) Organizing committee of the CARISMA-COST meeting 2015, Tarragona (Spain), organized by COST-CARISMA and ICIQ.
- 8) Organizing committee of the EcostBio (Explicit control Over Spin States in Technology and Biochemistry) 2014, organized by IQCC (Institute of Computational Chemistry and Catalysis) and University of Girona (UdG).

**Attendance:** 71<sup>st</sup> Lindau Nobel Laureate meeting 2022, KVC Photo-Cat Symposium 2021, Chemical Science biohybrids symposium 2021, 9<sup>th</sup> SFN symposium, JBIC online seminar 2021, KTN Online seminar (2020-2021), Online 8<sup>th</sup> SFN symposium (January 2021), Global Young Scientist Submit January 2021 (GYSS) in Singapore upon invitation (online), ICIQ Symposium Lights on Chemistry 2015.

**Invited to the 71<sup>st</sup> Lindau Nobel Laureate Meeting in Chemistry 2022.**

#### 13. Outreach activities

- **July 2023:** Co-PI in the successful outreach project “Joves I Ciència 2023 – project Artificial Photosynthesis”- teaching and outreach summer campus for “A levels students” during two weeks in July in a science summer camp.
- **May-June 2023:** member of the Inspira STEAM 2023 team – giving 3 sessions (2h lectures and activities) at schools to promote scientific vocations among kids and teenagers.
- **February 2023:** Talk on the international day of women and girls in science at ICIQ.
- **Sept. 2022:** talk at Cosmocaixa Tarragona 2022: “Artificial Photosynthesis: from solar fuels to solar chemicals”.
- **Sept. 2022:** researcher’s night 2022: experiments and talks in Tarragona.

- **July 2022:** Co-PI in the successful outreach project “Joves I Ciència 2022 – project Artificial Photosynthesis”- teaching and outreach summer campus for “A levels students” during two weeks in July in a science summer camp.
- **March 2021:** “Mujeres con química” video to promote the importance of diversity and the role of women in science and specially in chemistry.
- **March 2021:** Virtual Science Festival 2021 from the Univ. Cambridge; <https://www.ch.cam.ac.uk/outreach>.
- **March 2021:** #100tifiques – #100tifiques – set of online outreach talks at schools (2 talks total in 8 courses) during the week of women in science ([https://100tifiques.cat/en/100tifiques-2021\\_en/](https://100tifiques.cat/en/100tifiques-2021_en/)).
- **March 2017:** Cosmocaixa Lleida: outreach talk about “Solar fuels and Artificial photosynthesis”.
- **March 2017:** Contribution in an outreach article in “Chemistry World” (Y viva Tarragona: <https://www.chemistryworld.com/careers/fancy-a-job-in-tarragona-spain/2500271.article>).
- **2009-2012:** Science divulgation in the Chemistry department (“Researchers Night” and other events) at UdG.

#### 14. Research Summary and main scientific achievements

I am currently a Ramón y Cajal fellow and a Junior Group Leader at the University Rovira i Virgili (URV) and the Institute of Chemical Research of Catalonia (ICIQ) in Tarragona (Spain). [My group](#) focuses on the development and study of catalyst-functionalized polymeric microreactors (polymersomes) for solar fuels and chemicals, with the aim to compartmentalize and separate oxidation and reduction reactions, within artificial photosynthesis. This research lies at the interface of chemistry, material science, homogeneous and heterogeneous catalysis and aims to develop new conceptual design in the field of artificial photosynthesis and advance in the knowledge of reactivity in confined spaces and interfaces.

My career began at the University of Girona (Spain) as a MSc student under the supervision of Prof. Miquel Costas and Prof. Julio Lloret-Fillol (2013–2014), developing molecular Ru complexes for water and C-H oxidation. Then I moved to ICIQ to do the PhD (FPU fellowship, 2015-2019) in the group of Prof. J. Lloret-Fillol working on the understanding of AP mechanisms. In this line, I worked in the development and study of well-defined Fe and Ru complexes for water oxidation and a Co/Cu dual photocatalytic system for light-driven organic methodology (photoredox catalysis). Moreover, I did 4 PhD internships to learn new techniques, expand my scientific knowledge and establish collaborations: a) KTH Sweden (Prof. M. Ahlquist) calculations of EPR spectra; b) ASU US (Prof. G. Ghirlanda, 3 months) metalloenzymes for water reduction/oxidation (*Catalysts* 2021 corresponding author; *ACS Catal* 2019); c) Univ. Groningen Netherlands (Prof. W. R. Browne, 15 days) Raman spectroscopy (*Nat Chem* 2021); d) MPI-CEC Germany (Prof. S. DeBeer, Dr. O. Rüdiger, 1 month) EPR spectroelectrochemistry and XAS (*ChemElectroChem* 2021). In September 2019 I joined the group of Prof. E. Reisner (University of Cambridge) as BBSRC postdoc to develop biohybrid systems for solar fuels, and C-based materials for organic methodology. From Oct. 2020-Sept. 2022 I was a Marie Skłodowska Curie Fellow in the same group, interfacing enzymes with synthetic photocatalysts for CO<sub>2</sub> and water reduction. I have a very unique multidisciplinary background with experience in organic/inorganic synthesis, (photo)catalysis, material science and reaction mechanisms (spectroscopy, electrochemistry, DFT) with homo- and heterogeneous systems, and enzymes. Main scientific contributions to the field of AP:

- **Homogeneous water oxidation:** development of well-defined Fe and Ru complexes for WO and their mechanistic study (*ACS Catal* 2021; *AINC* 2019; *JACS* 2019). Characterization of intermediates led to comprehensive understanding of the generation and stabilization of high valent M-oxo species and a direct activity comparison between analogous Ru and Fe complexes (*ChemElectroChem* 2021; *Chem Eur J* 2016). A breakthrough in the field was the 1<sup>st</sup> direct proof of the O-O bond formation via water nucleophilic attack, which was questioned since the 80s. This was possible because I isolated 2 reaction intermediates, 1 before the RDS (O-O bond formation) and the other after, allowing to track the origin of the O-O during the formation of O<sub>2</sub> when they are still bound to the metal center (*Nat Chem* 2021).
- **Homogeneous light-driven organic substrate and water reduction:** Development and study of a dual Co/Cu photocatalytic system for the reduction of aromatic ketones, aldehydes, and aromatic olefins under visible light in aqueous media. Detailed mechanistic understanding allowed for rational design of the reaction conditions to tune the selectivity toward olefin reduction (100%) in presence of ketones and *vice versa* (*Chem. Sci.* 2022, Cover; *Chem Sci* 2017, Cover). This was possible thanks to the development of *in house* parallel photoreactors during my PhD (*ACS Symposium Series* 2022, patented and licensed to [Trellum Technologies](#) for industrialization). Study of the 2<sup>nd</sup> coordination sphere upon biotinylation of Co complexes and encapsulation into Streptavidin, showing increased photo- and electrocatalytic activity for WR (*Catalysts* 2021; *ACS Catal* 2019). Characterization of a low valent Co(I) (*JACS* 2020).
- **Biohybrids for AP:** I introduced a new research line at the ReisnerLab: surface modification of carbon dots (CDs) for labelling of proteins, enzymes and molecular catalysts for AP. I developed a new strategy to modify CDs with a maleimide derivative for site-specific labelling of a transmembrane cytochrome MtrC protein from non-photosynthetic *S. oneidensis* bacterium to invert the microbial electron flow, and drive the electrons from the oxidation site (CD) to the inside of the microorganism to engage with redox enzymes for fuel production (*Adv. Funt. Mat.* 2023). CD-MtrC system was also used to study membrane electron transfer in proteoliposomes for photocatalytic dye degradation and removal of N<sub>2</sub>O (*ACIE* 2022, *Chem. Soc. Rev.* 2021; *Front. Microbiol.* 2021). Then we interfaced

CDs and CNTs with formate dehydrogenase enzymes to establish enzyme orientation principles for photo- and electroreduction of CO<sub>2</sub> ([JACS 2022](#)).

- C-based materials for photoredox catalysis: deconvolution of the sizes in bulk CDs and study of the size-effect for H<sub>2</sub> production ([Nanoscale 2023](#)). Sustainable organic methodology: i) single atom photocatalysis with Ni-doped carbon nitride for C-N and C-O coupling, ii) metal-free carbon nitride for, and azolation reactions ([ACIE 2022](#), [ChemSusChem 2021](#); [ACIE 2021](#)).