Enric Petrus Pérez

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(curriculum vitae, November 2024)

Academic Record

2023 June - ongoing	**Postdoctoral fellow**, Swiss Federal Institute of Aquatic Science and Technology Eawag (Dübendorf, Switzerland) Supervisor: PD. Dr. Thomas B. Hofstetter (thomas.hofstetter@eawag.ch)
2022 Dec - 2023 May	**Postdoctoral fellow**, Institute of Chemical Research of Catalonia ICIQ (Tarragona, Spain) Supervisor: Prof. Carles Bo (cbo@iciq.cat)
2021 Sep-Dec	**International Secondment during the PhD**, Swiss Federal Institute of Technology ETH (Zürich, Switzerland) Supervisor: Prof. Markus Reiher (markus.reiher@phys.chem.ethz.ch)
2018-2022	**International PhD in Technology and Science**, Roviri i Virgili University URV and Institute of Chemical Research of Catalonia ICIQ (Tarragona, Spain) Doctoral Thesis title: *POMSimulator: a Method for Understanding the Multi-Equilibria and Self-Assembly Processes of Polyoxometalates* Supervisor: Prof. Carles Bo (cbo@iciq.cat)
2017-2018	**Master in Synthesis, Catalysis and Molecular Design**, Roviri i Virgili University URV and Institute of Chemical Research of Catalonia ICIQ (Tarragona, Spain) Master Thesis title: *Computational Modelling of Uranyl Complexes* Supervisor: Prof. Carles Bo (cbo@iciq.cat)
2013-2017	**Chemistry Degree**, Roviri i Virgili University URV (Tarragona, Spain)

Research Publications

1. Martin, N. P.; Petrus, E.; Segado, M.; Arteaga, A.; Zakharov, L. N.; Bo, C.; Nyman, M. Strategic Capture of the {Nb7} Polyoxometalate. *Chem. - A Eur. J.* **2019**, 10580–10584. DOI
2. Petrus, E.; Bo, C. Performance of Group Additivity Methods for Predicting the Stability of Uranyl Complexes. *J. Comput. Chem.* **2020**, 41, 11, 1124–1129. DOI
3. Petrus, E.; Segado, M.; Bandeira, N. A. G.; Bo, C. Unveiling a Photoinduced Hydrogen Evolution Reaction Mechanism via the Concerted Formation of Uranyl Peroxide. *Inorg. Chem.* **2020**, 59, 12, 8353–8360. DOI
4. Petrus, E.; Segado, M.; Bo, C. Nucleation Mechanisms and Speciation of Metal Oxide Clusters. *Chem. Sci.* **2020**, 11, 8448-8456. DOI; *Preprint Available at chemrxiv*
5. Petrus, E.; Bo, C. Unlocking Phase Diagrams for Molybdenum and Tungsten Nanoclusters and Prediction of their Formation Constants. *J. Phys. Chem. A* **2021**, 125, 23, 5212–5219. DOI; *Preprint Available at chemrxiv*

6. Rahman, T.; Petrus, E.; Segado, M.; Martin, N. P.; Palys, L. N.; Rambaran, M. A.; Ohlin, A.; Bo, C.; Nyman, M. Predicting the Solubility of Inorganic Ion Pairs in Water *Angew. Chem. Int. Ed.* **2022**, 61, e202117839; DOI
7. Petrus, E.; Segado, M.; Bo, C. Computational Prediction of Speciation Diagrams and Nucleation Mechanisms: Molecular Vanadium, Niobium and Tantalum Oxide Nanoclusters in Solution *Inorg. Chem.* **2022**, 61, 35, 13708–13718. DOI; *Preprint Available at chemrxiv*
8. Garay-Ruiz, D.; Petrus, E.; Bo, C. New graph-based computational methods for dealing with chemical reactivity and catalysis *Revista de la Societat Catalana de Quimica*, **2023**, 22, 23-38; DOI
9. Petrus, E.; Garay-Ruiz, D.; Reiher, M.; Bo, C. Multi-Time-Scale Simulation of Complex Reactive Mixtures: How Do Polyoxometalates Form? *J. Am. Chem. Soc.* **2023**, 145, 34, 18920-18930; DOI
10. Tamai, N.; Ogiwara, N.; Hayashi, E.; Kamata, K.; Misaya, T.; Ito, T.; Kojima, T.; Segado, M.; Petrus, E.; Bo, C.; Uchida, S. A redox-active inorganic crown ether based on a polyoxometalate capsule *Chem. Sci.* **2023**, 14, 20, 5453-5459; DOI
11. Petrus, E.; Builes, J.; Garay-Ruiz, D.; Segado-Centellas, M.; Bo, C. POMSimulator: An open-source tool for predicting the aqueous speciation and self–assembly mechanisms of polyoxometalates *J. Comput. Chem.* **2024**, 45, 2242–2250; DOI
12. Builes, J.; Garay-Ruiz, D.; Segado-Centellas, M.; Petrus, E.; Bo, C. Computational insights into aqueous speciation of metal-oxide nanoclusters: an in-depth study of the Keggin phosphomolybdate *Chem. Sci.* **2024**, 15, 14218-14227; DOI
13. Builes, J.; Garay-Ruiz, D.; Petrus, E.; Segado-Centellas, M.; Bo, C. Towards a Universal Scaling Method for Predicting Equilibrium Constants of Polyoxometalates. ChemRxiv **2024**; DOI

Congresses & Outreach

1. Poster Presentation: *Unveiling a Photoinduced Hydrogen Evolution Reaction Mechanism via the Concerted Formation of Uranyl Peroxide* – INTECAT School **2018** (Riudoms, Spain)
2. Poster Presentation: *Unveiling a Photoinduced Hydrogen Evolution Reaction Mechanism via the Concerted Formation of Uranyl Peroxide* – ICIQ PhD Day **2019** (Tarragona, Spain)
3. Outreach Talk (monologue): *"Vols saber que investigo? Urani, t'excites?"* – URV **2019** (Reus, Spain) url: https://www.youtube.com/watch?v=afLn5BxYf7U (accessed 10/03/23)
4. Poster Presentation: *Unveiling a Photoinduced Hydrogen Evolution Reaction Mechanism viathe Concerted Formation of Uranyl Peroxide* – Frontiers in Metal Oxide Cluster Science VI **2019**(Corvailis, USA)
5. Oral Communication: *Performance of group additivity methods for predicting the stability of uranyl complexes* – Conference of the Catalan Society of Chemistry **2020** (Sitges, Spain)
6. Outreach Talk (radio program): *La química computacional* – Ones de Ciència Cambrils **2020**, (Cambrils, Spain) url: https://www.radiocambrils.cat/programs/ones-de-ciencia/radiocambrils_podcast_2244 (accessed 10/03/23)
7. Flash Presentation: *Speciation and Self-Assembly Mechanism of Polyoxometalates* – ICIQ PhD Day **2020** (Tarragona, Spain)
8. Conference Organizer: ICIQ PhD Day **2022** – (Tarragona, Spain)
9. Oral Communication: *Mecanismes de Formació i Diagrames d'Especiació dels Òxids Metàl·lics Moleculars* – Conference of the Catalan Society of Chemistry **2022** (Girona, Spain)

10. Oral Communication: *POMSimulator: a Method for Predicting the Speciation and Self-Assembly of Polyoxometalates* – International Conference of Coordination Chemistry **2022** (Rimini, Italy)
11. Outreach Talk (presentation): *La intel·ligència artificial un futur ple de transformacions* – European Night of Research **2022** (Reus, Spain) url: https://www.youtube.com/watch?v=EGGs6VePeJo&list=PL4Rm01OU_6h5xwodLDGQIOkbk_Mrl8dJe&index=9 (accessed 10/03/23)
12. Oral Communication: *Predicting the aqueous speciation and self-assembly mechanisms of Mo, W, V, Nb and Ta polyoxometalates* – Reunió de Química Inorgànica I Organometàl·lica **2023** (Barcelona, Spain)
13. Oral Communication: *Ten years of interplay between theory and experiments* – ACS Spring **2023** (Indianapolis, USA)
14. Oral Communication: *Development of a Method for Predicting the Aqueous Speciation and Self-Assembly of Polyoxometalates* – Frontiers in Metal Oxide Cluster Science VII **2023** (Tarragona, Spain)
15. Workshop Organizer: *Introduction to Computational Chemistry* – NPOMs Computational Chemistry Workshop URV **2023** (Tarragona, Spain)
16. Poster Presentation: *Automated Reaction Network Exploration of Ozonation Processes in Water Treatment* – Swiss Chemical Society Fall Meeting **2023** (Bern, Switzerland)
17. Poster Presentation: *Automated Reaction Network Exploration of Ozonation Processes in Water Treatment* – 59th Symposium on Theoretical Chemistry **2023** (Zürich, Switzerland)
18. Poster Presentation: *Automated Reaction Network Exploration of Ozonation Processes in Water Treatment* – Eawag Symposium **2023** (Dübendorf, Switzerland)
19. Oral Communication: *An Open-Source Methodology for Predicting the Aqueous Speciation: from Polyoxometalates to Environmental Chemistry* – Electronic Structure Principles and Applications **2024** (Tarragona, Spain)
20. Poster Presentation: *Automated Reaction Network Exploration of Ozonation Processes in Water Treatment* - Gordon Research Conference (GRC) Computational Chemistry **2024** (Portland Maine, United Stated)
21. Oral Communication: *Automated Reaction Network Exploration of Ozonation Processes in Water Treatment* - SCS Fall Meeting **2024** (Fribourg, Switzerland)
22. Poster Presentation: *Automated Reaction Network Exploration of Ozonation Processes in Water Treatment* - ETH-Microsoft Workshop on High-Throughput Computational Chemistry **2024** (Zürich, Switzerland)
23. Poster Presentation: *Automated Reaction Network Exploration of Ozonation Processes in Water Treatment* - Eawag Symposium **2024** (Dübendorf, Switzerland)

Awards and Achievements

- Secondary Award for the Baccalaureate Final Project – Reddis Private Foundation **2014** (Reus, Spain)
- Secondary Award for the Degree Final Project – Catalan Society of Chemistry **2018** (Barcelona, Spain)
- First Award for the Scientific Monologue Competition – Roviri i Virgili University **2019** (Reus, Spain)
- First Award for the Best Oral Communication – ICIQ PhD Day **2020** (Tarragona, Spain)
- Cover Art for the J. Phys. Chem. A. **2021**, 125, 23, 5212-5219
- Highlight of three of our papers (Chem. Sci 2020, Inorg. Chem 2020, JACS 2023) on the official page of the *Software Chemistry & Material - Amsterdam Density Functional*
- ICIQ Fellowship for the Master "Synthesis, Catalysis and Molecular Design" **2017** (Tarragona, Spain)
- ICIQ Fellowship for the PhD in Science and Technology **2018** (Tarragona, Spain)

- Severo Ochoa Fellowship for a secondment at ETH Zürich **2021** (Tarragona, Spain).
- Reviewer in the Journal of Computational Chemistry (Wiley) and Inorganic Chemistry (ACS) – **2022-onwards**
- Cum Laude Mention and International Doctoral Mention – Rovira i Virgili University **2022** (Tarragona, Spain)
- Cover Art for the JACS **2023**, 145, 34, 18920-18930
- First Award for the Poster Presentation – Eawag Symposium **2023** (Dübendorf, Switzerland)
- First Award for the III Computational Methodology Prize by the Chemistry Computation Division of the Spanish Royal Society of Chemistry **2023** (Madrid, Spain)

Skills

- Languages: English (C1), French (B2), German (B1) and native in Spanish and Catalan
- Advanced knowledge in Bash, Python Programming Language, Mongo-DB, C++ and machine learning algorithms
- Intermediate user in 3D design with Blender
- Experience in commercial programs based on quantum mechanics for chemical systems (Amsterdam Density Functional, Gaussian, ORCA)