JORDI BUILS

P.h.D in Computational Chemistry

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EXPERIENCE

Postodctoral Researcher

Prof. Carles Bo Jané - Institute of Chemical Research of Catalonia (ICIQ)

December 2024 - Currently

Tarragona, Spain

EDUCATION

P.h.D Degree in Chemical science and Technology (Cum Laude and International Mention)

Prof. Carles Bo Jané and Dr. Mireia Segado Centellas at Institute of Chemical Research of Catalonia (ICIQ)

November 2021 - December 2024

Tarragona, Spain

Master Degree in Chemical Science and Technology

Prof. Àngel Terrón Homar - University of the Balearic Islands

September 2020 - September 2021

Mallorca, Spain

Bachelor Degree in Chemistry

Prof. Àngel Terrón Homar - University of the Balearic Islands

September 2015 - February 2020

Mallorca, Spain

Skills

- **Density Functional Theory code:** ADF (Amsterdam Density Functional, AMS (Amsterdam Modeling Suite) Gaussian
- Programming Languages: Python, Bash
- Libraries: Scipy, Numpy, Pandas, Scikit-Learn, PyTorch
- Open data: Git (GitLab and GitHub), ioChem-BD
- Languages: Catalan, Spanish, and English

Open Sourced projects

POMSimulator 1.0.0 : Chemistry toolkit for simulating the aqueous speciation of metal-oxo clusters

https://github.com/petrusen/pomsimulator

POMSimulator 2.0.0: Chemistry toolkit for simulating the aqueous speciation of metal-oxo clusters

https://github.com/petrusen/pomsimulator

POMs-GibbsNet : A DNN model for the prediction of thermodynamic properties of metal-oxo clusters

https://gitlab.com/jbuils/poms-gibbsnet

POMs DataBase: A collection of metal-oxo clusters for the training of GibbsNet

ioChem-bd

Publications

- F. Ibrahima Bamba, C. Falaise, N. Leclerc, M. Haouas, G. Gbassi, P. Atheba, M. Fregnaux, **J.Buils**, M. Segado-Centellas, C. Bo, E. Cadot. "Capping the Electronic Lone Pair of the As(III) Central Atom in the Keggin-type Anion: From Experimental-Theoretical Interplay to Evidence." Inorganic Chemistry **(2025)**
- J. Bustos, M. Shohel, A. G. Buzanich, L. Zakharov, **J. Buils**, M. Segado-Centellas, C. Bo, M. Nyman. "Thechnetium and Rhenium Auto-reduction, Polimerization and Lability towards Group VII Polyoxometalate Chemistry." Chemistry-A European Journal 31, 21 **(2025)**
- **J. Buils**, D. Garay-Ruiz, E. Petrus, M. Segado-Centellas, C. Bo. "Towards a universal scaling method for predicting equilibrium constants of polyoxometalates." Digital Discovery, 4, 4, 970-978 **(2025)**
- D. Garay-Ruiz, **J. Buils**, N. A. G. Bandeira, S. Floquet, E. Cadot, C. Bo. "Thinking about the Box: Exploring the Electronic Structure of Cuboidal-Shaped Mo_{84} Anionic Nanocapsule." Inorganic Chemistry **(2025)**
- **J. Buils**, D. Garay-Ruiz, E. Petrus, M. Segado-Centellas, C. Bo. "Computational insights into aqueous speciation of metal-oxide nanoclusters: an in-depth study of the Keggin phosphomolybdate." Chemical Science, 15, 35, 14218-14227 **(2024)**
- E. Petrus, **J. Buils**, D. Garay-Ruiz, M. Segado-Centellas, C. Bo. "POMSimulator: An open-source tool for predicting the aqueous speciation and self-assembly mechanisms of polyoxometalates." Journal of Computational Chemistry, 45, 26, 2242-2250 **(2024)**
- D. Cebotari, **J. Buils**, O. Garbuz, G. Balan, J. Marrot, V. Guérineau, D. Touboul, M. Haouas, M. Segado-Centellas, C. Bo, A. Gulea, S. Floquet. " A new series of $Mo(V)_2O_2S_2$-based thiosemicarbazone complexes: Solution and DFT studies, and antifungal and antioxidant activities." Journal of Inorganic Biochemistry, 245 **(2023)**
- M. De las Nieves-Piña, S. Burguera, **J. Buils**, M. A. Crespi, J. E. Morales, J. Pons, A. Bauzá, A. Frontera. "Substituen Effects in π-Hole Regium Bonding Interactions Between $Au(p\text{-}X\text{-}Py)_2$ Complexes and Lewis Bases: An ab initio Study." ChemPhysChem, 23, 8 **(2022)**
- A. Terrón, **J.Buils**, T. J. Mooibroek, M. Barceló-Oliver, A. García-Raso, J.J. Fiol, A. Frontera "Synthesis, X-ray characterization and regium bonding interactions of a trichlorido (1-hexylcytosine) gold(III) complex." Chemical Communications, 56, 24, 3524-3527 **(2020)**

Conferences

- **J.Buils**, E. Petrus, D. Garay-Ruiz, M. Segado-Centellas, C. Bo. **(2025)** "Predicció de l'especiació aquosa de heteropolioxometal·lats: el fosfomolibdat i l'arsenomolibdat." Oral comunication (flash) at "2ª Reunió de Química Inorgànica i Organometàl·lica de la SCQ", Tarragona, Spain
- **J.Buils**, E. Petrus, D. Garay-Ruiz, M. Segado-Centellas, C. Bo. **(2024)** "DFT Simulations of Complex Reaction Networks to solve the aqueous speciation of polyoxometalates" Oral comunication (flash) + poster at "EuChemS 2024", Dublin, Ireland
- **J.Buils**, E. Petrus, D. Garay-Ruiz, M. Segado-Centellas, C. Bo. **(2024)** "DFT Simulations of Complex Reaction Networks to solve the aqueous speciation of polyoxometalates" Oral comunication (flash) at "ESPA 2024", Tarragona, Spain
- **J.Buils**, E. Petrus, D. Garay-Ruiz, M. Segado-Centellas, C. Bo. **(2024)** "Simulacions de Xarxes de Reacció Complexes d'Òxids de Molibdé." Oral comunication (flash) at "13ª Trobada de Joves Investigadors dels Països Catalans", Tarragona, Spain
- **J.Buils**, E. Petrus, D. Garay-Ruiz, M. Segado-Centellas, C. Bo. **(2023)** "DFT Simulations of Complex Reactoin Networks: Aqueous speciation of Molybdenum Oxides and Formation of the Keggin anion." Poster comunication at "EuChemS CompChem 2023", Thessaloniki, Greece
- **J.Buils**, E. Petrus, D. Garay-Ruiz, M. Segado-Centellas, C. Bo. **(2023)** "DFT Simulations of Complex Reactoin Networks: Aqueous speciation of Molybdenum Oxides and Formation of the Keggin anion." Oral communication at "XXXIX Reunión Bienal de la Sociedad Española de Química", Zaragoza, Spain
- **J.Buils**, E. Petrus, M. Segado-Centellas, C. Bo. **(2023)** "Understanding the aqueous speciation of heteropolyoxometalates with POMSimulator: the Keggin anion." Oral communication (flash) at "Frontiers in metal oxide cluster science", Tarragona, Spain
- **J.Buils**, E. Petrus, M. Segado-Centellas, C. Bo. **(2023)** "POMSimulator: Estudiant el mecanisme de formació de l'anió Keggin en solució aquosa" Poster communication at "1ª Reunió de Química Teòrica i Computacional de la SCQ", Barcelona, Spain
- **J.Buils**, E. Petrus, M. Segado-Centellas, C. Bo. **(2022)** "On the use of the POMSimulator to understand the formation mechanism of metal oxide nanoclusters: the Keggin anion" Poster communication at "VI PhD Day", Tarragona, Spain
- **J.Buils**, E. Petrus, M. Segado-Centellas, C. Bo. **(2022)** "On the use of the POMSimulator to understand the formation mechanism of metal oxide nanoclusters: the Keggin anion" Poster communication at "VI PhD Day", Rimini, Italy
- **J.Buils**, E. Petrus, M. Segado-Centellas, C. Bo. **(2022)** "On the use of the POMSimulator to understand the formation mechanism of metal oxide nanoclusters: the Keggin anion" Poster communication at "Summer School in Polyoxometalates Chemistry for Fundamentals and Applications", La Rochelle, France

Workshops and courses

- Using the Amsterdam Modeling Suite in HPC Systems. Organized by SCM AMS **(2022)** Online 16h
- Skibotn hackathon at Trömso **(2024)** presential 4 days

Supervision and mentoring

- Mentoring of Dr. L. Susanne Junkers. University of Copenhagen
  During three months of her P.h.D secondment, supervised her use of POMSimulator to adapt it to thermosynthesis conditions.
  (2024)
- Supervision of Ms Farzaneh Hosseini. Institute of Chemical Research of Catalonia
  Since start of her P.h.D, supervised her adaptation to the group working line. Adaptation of POMSimulator to her project needs.
  (2025)