1) Personal information

Personal details	
First Name, Last Name: Jordi, Builds Casasnovas	**DNI:** 43203996-Z
Citizenship: Spanish	**Phone Number:** +34 671761911
Date of Birth (dd/mm/yyyy): 26/04/1997 **Place of Birth:** Palma de Mallorca (Spain)	**e-mail:** jbuils@iciq.es jordibuils@gmail.com
Scientific identification	
ORCID	0000-0002-2674-6551
Google Scholar	Link
Current Position	**Date (dd/mm/yyyy)**
Postdoctoral Researcher at the Institute of Chemical Research of Catalonia (ICIQ)	21/12/2024 - Currently

2) Scientific trajectory

I am a **computational chemist** from Mallorca, Spain. I began my academic journey by earning a Bachelor's Degree in Chemistry from the University of the Balearic Islands. During this period, I developed a strong interest in **inorganic chemistry** and **computational inorganic chemistry**, which led me to pursue a Master's Degree in Chemical Science and Technology at the same institution, where I had the opportunity to work under the supervision of **Prof. Àngel Terrón Homar**.

Driven by my growing interest in theoretical modelling, I started my PhD in Chemical Science and Technology at Rovira i Virgili University (URV), in the Inorganic and Physical Chemistry Department. My doctoral research, supervised by **Prof. Carles Bo Jané and Dr. Mireia Segado Centellas**, focused on **polyoxometalates (POMs)** was entitled **“Enhancing POMSimulator Applications in Heteropolyoxometalates: A Statistical and Data-Driven Approach”**. I successfully defended my thesis in December 2024, earning an **"Excellent Cum Laude"** distinction along with the International Mention.

During my PhD, I became deeply involved in the development of **open-source** tools for the modelling of polyoxometalates. I contributed

significantly to the development of **POMSimulator**, a tool for predicting aqueous speciation and self-assembly mechanisms of POMs. I also led the development of **POMs-GibbsNet**, a platform that combines DFT results with deep neural networks for thermodynamic property predictions. In this same project, I generated a database containing **thousands of polyoxometalates**.

In early 2024, I completed a three-month international research stay at the University of Oslo, working in the **Hylleraas Centre of Excellence for Quantum Molecular Sciences** under the guidance of **Prof. David Balcells**. There, I explored the integration of machine learning algorithms with DFT calculations to predict the thermodynamic properties of polyoxometalates—an experience that expanded my expertise in data science and its applications in theoretical chemistry, leading to the development of the **POMS-GibbsNet**.

After completing my PhD, I continued at ICIQ as a **postdoctoral researcher**, where I am currently working. My research has focused on the simulation of **complex reaction networks** in **aqueous environments**, particularly involving molybdenum-based POMs. I have authored nine peer-reviewed articles, including **five in Q1 journals**, with one being recognized as an **"Editor's Choice"**. My work has attracted more than 60 citations and contributed to advancing computational methods in **inorganic chemistry**.

Throughout my academic journey, I have presented my research in numerous **national and international conferences**, including EuChemS, ESPA or ICCC. I have also contributed to competitive national research projects, such as those funded by the Spanish Ministry of Science and the Severo Ochoa Excellence Program. Furthermore, I have supervised and mentored early-career researchers, including PhD students conducting secondments at ICIQ.

My scientific career has been shaped by a strong foundation in **computational and inorganic chemistry**, a passion for **open science**, and a commitment to advancing our understanding of **complex molecular systems** through interdisciplinary collaboration.

3) Education

Phd: Chemical Science and Technology	
University	Inorganic and physics department, Rovira i Virgili University (URV)
Supervisors:	Prof. Carles Bo Jané Dr. Mireia Segado Centellas
Title of PhD Thesis	Enhancing POMSimulator Applications in Heteropolyoxometalates: A Statistical and Data-Drive Approach
Qualification	Excellent, Cum Laude – International Mention
Date (dd/mm/yyyy)	20/12/2024

Master's degree: Chemical Science and Technology	
University	Chemistry department, University of the Balearic Islands
Supervisors:	Prof. Angel Terrón Homar
Title of MSc Thesis	
Qualification	
Date (dd/mm/yyyy)	

Bachelor's Degree: Chemistry	
University	Chemistry department, University of the Balearic Islands
Supervisors:	Prof. Angel Terrón Homar
Title of BSc Thesis	
Date (dd/mm/yyyy)	

Language knowledge:

Catalan: Spoken (Native) Reading (Native) Written (Native)

Spanish: Spoken (Native) Reading (Native) Written (Native)

English: Spoken (Very good) Reading (Very good) Written (Very good)

4) Past and current position

Pre-doctoral researcher
Centre: Institute of Chemical Research of Catalonia (Tarragona, Spain) **Supervisors:** Prof. Carles Bo and Dr. Mireia Segado-Centellas **Date:** Nov-2021 --- Dec-2024

Postdoctoral researcher
Centre: Institute of Chemical Research of Catalonia (Tarragona, Spain) **Supervisors:** Prof. Carles Bo **Date:** Dec-2024 --- Currently

5) Research activities

a) Scientific Publications

Summary of my scientific publications and bibliometric details:

TYPE	**NUMBER**
TOTAL ARTICLES	9
1ST AUTHOR ARTICLES	2
ARTICLES IN Q1 JOURNALS	5
"EDITOR'S CHOICE"	1
TOTAL CITATIONS (GOOGLE SCHOLAR)	62
INDEX H (GOOGLE SCHOLAR)	4
INDEX I10 (GOOGLE SCHOLAR)	1

Scientific publications from more recent to older:

1	**Type:** Article
	Authors: F. I. Bamba, C. Falaise, N. Leclerc, M. Haouas, G. Gbassi, P. Atheba, M. Fregnaux, **Jordi Buils**, M. Segado-Centellas, C. Bo, E. Cadot
	Title: Capping the electronic lone pair of the As(III) central atom in the Keggin-type anion. From experimental – theoretical interplay to evidence
	Year: 2025
	Journal: Inorganic Chemistry

	DOI: NO DOI YET
	Category and Quartile (JCR, SCIE): Chemistry, Inorganic & Nuclear (Q1, 8/44)
	Impact Factor: 4.1
	Citations: -

2	**Type:** Article
	Authors: J. Bustos, M. Shohel, A. G. Buzanich, L. Zakharov, **Jordi Builds,** M. Segado-Centellas, C. Bo, M. Nyman
	Title: Technetium and Rhenium Auto-reduction, Polymerization and Lability towards Group VII Polyoxometalate Chemistry
	Year: 2025
	Journal: Chemistry-A European Journal
	DOI: 10.1002/chem.202404144
	Category and Quartile (JCR, SCIE): Chemistry, Multidisciplinary (Q2, 80/231)
	Impact Factor: 4.1
	Citations: 1

3	**Type:** Article
	Authors: Jordi Builds, D. Garay-Ruiz, E. Petrus, M. Segado-Centellas, C. Bo
	Title: Towards a universal scaling method for predicting equilibrium constants of polyoxometalates
	Year: 2025
	Journal: Digital Discovery
	DOI: 10.1039/d4dd00358f
	Category and Quartile (JCR, SCIE): Computer Science, Interdisciplinary Applications (Q1, 25/170)
	Impact Factor: 6.2
	Citations: -

4	**Type:** Article
	Authors: D. Garay-Ruiz, **Jordi Builds**, N. A. Bandeira, S. Floquet, E. Cadot, C. Bo
	Title: Thinking about the Box: Exploring the Electronic Structure of a Cuboidal-Shaped Mo84 Anionic Nanocapsule
	Year: 2025

	Journal: Inorganic Chemistry
	DOI: 10.1021/acs.inorgchem.4c04497
	Category and Quartile (JCR, SCIE): Chemistry, Inorganic & Nuclear (Q1, 8/44)
	Impact Factor: 4.1
	Citations: -

5	**Type:** Article
	Authors: **Jordi Buils**, D. Garay-Ruiz, M. Segado-Centellas, E. Petrus, C. Bo
	Title: Computational insights into aqueous speciation of metal-oxide nanoclusters; an in-depth study of the Keggin phosphomolybdates
	Year: 2024
	Journal: Chemical Science
	DOI: 10.1039/d4sc03282a
	Category and Quartile (JCR, SCIE): Chemistry, Multidisciplinary (Q1, 40/231)
	Impact Factor: 8
	Citations: 2

6	**Type:** Article
	Authors: E. Petrus, **Jordi Buils**, D. Garay-Ruiz, M. Segado-Centellas, C. Bo
	Title: POMSimulator: An open-source tool for predicting the aqueous speciation and self-assembly mechanisms of polyoxometalates
	Year: 2024
	Journal: Journal of Computational Chemistry
	DOI: 10.1002/jcc.27389
	Category and Quartile (JCR, SCIE): Chemistry, Multidisciplinary (Q2, 93/231)
	Impact Factor: 3.7
	Citations: 4

7	**Type:** Article
	Authors: D. Cebotari, **Jordi Builds**, O. Garbuz, G. Balan, J. Marrot, V. Guerineau, D. Touboul, M. Haouas, M. Segado-Centellas, C. Bo, A. Gulea, S. Floquet
	Title: A new series of bioactive Mo(V)2O2S2-based thiosemicarbazone complexes: Solution and DFT studies, and antifungal and antioxidant activities
	Year: 2023
	Journal: Journal of Inorganic Biochemistry
	DOI: 10.1016/j.jinorgbio.2023.112258
	Category and Quartile (JCR, SCIE): Chemistry, Inorganic & Nuclear (Q1, 10/44)
	Impact Factor: 3.5
	Citations: 5

8	**Type:** Article
	Authors: M. De las Nieves Piña, S. Burguera, **Jordi Builds**, M. A. Crespí, J. E. Morales, J. Pons, A. Bauza, A. Frontera
	Title: Substituent Effects in pi-Hole Regium Bonding Interactions Between Au(p-X-Py)2 Complexes and Lewis Bases: An ab initio Study
	Year: 2022
	Journal: ChemPhysChem
	DOI: 10.1002/cphc.202200010
	Category and Quartile (JCR, SCIE): Physics, Atomics, Molecular & Chemical (Q2, 16/40)
	Impact Factor: 2.8
	Citations: 9

9	**Type:** Article
	Authors: A. Terrón, **Jordi Builds**, T. J. Mooibroek, M. Barceló-Oliver, A. García-Raso, J. J. Fiol, A. Frontera
	Title: Synthesis, X-ray characterization and regium bonding interaxctions of a trichlorido(1-hexylcytosine)gold(III) complex
	Year: 2020
	Journal: Chemical Communications
	DOI: 10.1039/d0cc00505c
	Category and Quartile (JCR, SCIE): Chemistry, Multidisciplinary (Q2, 72/231)

	Impact Factor: 4.4
	Citations: 30

b) Open-source software

1	**Type:** Software
	Authors: Enric Petrus, **Jordi Buils**, Diego Garay-Ruiz
	Title: POMSimulator 1.0.0
	Year: 2024
	DOI: 10.5281/zenodo.10689769
	Contribution: General development, code refactoring and writing of user manual

2	**Type:** Software
	Authors: Enric Petrus, **Jordi Buils**, Diego Garay-Ruiz
	Title: POMSimulator 2.0.0
	Year: 2025
	DOI: 10.5281/zenodo.15301990
	Contribution: New method implementation, code refactoring and actualization of user manual

3	**Type:** DataBase
	Authors: Jordi Buils
	Title: POMs-GibbsNet
	Year: 2025
	DOI:
	Contribution: Generation of DFT calculations, and data curation

4	**Type:** Software
	Authors: Jordi Buils
	Title: POMs-GibbsNet
	Year: 2025
	URL: https://gitlab.com/JBuils/poms-gibbsnet
	Contribution: General code development, adaptation of AABBA source code, and implementation of DNN. Adaptation of POMSimulator source code.

c) Participation in National and International Congresses

1	**Authors: <u>Jordi Builds</u>**, Enric Petrus, Mireia Segado-Centellas, Carles Bo
	Title: On the use of the POMSimulator to understand the formation mechanism of metal oxide nanoclusters: the Keggin anion.
	Type of Contribution: Poster
	Congress: Summer School in Polyoxometalates Chemistry for Fundamentals and Applications
	Year: 2022
	Location: La Rochelle, França

2	**Authors: <u>Jordi Builds</u>,** Enric Petrus, Mireia Segado-Centellas, Carles Bo
	Title: On the use of the POMSimulator to understand the formation mechanism of metal oxide nanoclusters: the Keggin anion.
	Type of Contribution: Poster
	Congress: International Conference on Coordination Chemistry (ICCC2022)
	Year: 2022
	Location: Rimini, Itàlia

3	**Authors: <u>Jordi Builds</u>**, Enric Petrus, Mireia Segado-Centellas, Carles Bo
	Title: On the use of the POMSimulator to understand the formation mechanism of metal oxide nanoclusters: the Keggin anion.
	Type of Contribution: Poster
	Congress: VI PhD Day
	Year: 2022
	Location: Tarragona, Espanya

4	**Authors: <u>Jordi Builds</u>,** Enric Petrus, Mireia Segado-Centellas, Carles Bo
	Title: POMSimulator: Estudiant el mecanisme de formació de l'anió Keggin en solució aquosa.
	Type of Contribution: Poster

	Congress: 1a Reunió de Química Teòrica i Computacional de la SCQ
	Year: 2023
	Location: Barcelona, Espanya

5	**Authors: Jordi Builds**, Enric Petrus, Mireia Segado-Centellas, Carles Bo
	Title: Understanding the aqueous speciation of heteropolyoxometalates with POMSimulator: the Keggin anion.
	Type of Contribution: Flash communication
	Congress: Frontiers in metal oxide cluster science
	Year: 2023
	Location: Tarragona, Espanya

6	**Authors: Jordi Builds**, Enric Petrus, Diego Garay-Ruiz, Mireia Segado-Centellas, Carles Bo
	Title: DFT Simulation of Complex Reaction Networks: Aqueous speciation of Molybdenum Oxides and Formation of the Keggin anion.
	Type of Contribution: Oral communication
	Congress: XXXIX Reunión Bienal de la Sociedad Española de Química
	Year: 2023
	Location: Saragossa, Espanya

7	**Authors: Jordi Builds,** Enric Petrus, Diego Garay-Ruiz, Mireia Segado-Centellas, Carles Bo
	Title: DFT Simulation of Complex Reaction Networks: Aqueous speciation of Molybdenum Oxides and Formation of the Keggin anion
	Type of Contribution: Poster
	Congress: 14th European Conference on Computational and Theoretical Chemistry (EuChemS CompChem 2023)
	Year: 2023
	Location: Tesalónica, Grècia

8	**Authors: Jordi Builds,** Enric Petrus, Diego Garay-Ruiz, Mireia Segado-Centellas, Carles Bo
	Title: Simulacions de Xarxes de Reacció Complexes d'Òxids de Molibdé.

	Type of Contribution: Oral communication
	Congress: 13a Trobada de Joves Investigadors dels Països Catalans
	Year: 2024
	Location: Tarragona, Espanya

9	**Authors: Jordi Builds**, Enric Petrus, Diego Garay-Ruiz, Mireia Segado-Centellas, Carles Bo
	Title: DFT Simulation of Complex Reaction Network to solve aqueous speciation of polyoxometalates.
	Type of Contribution: Flash communication
	Congress: Electronic Structure Principles and Applications (ESPA24)
	Year: 2024
	Location: Tarragona, Espanya

10	**Authors: Jordi Builds**, Enric Petrus, Diego Garay-Ruiz, Mireia Segado-Centellas, Carles Bo
	Title: DFT Simulation of Complex Reaction Networks to solve aqueous speciation of polyoxometalates.
	Type of Contribution: Flash communication i Poster
	Congresss: EuChemS 2024
	Year: 2024
	Location: Dublin, Irlanda

11	**Authors: Jordi Builds**, Enric Petrus, Diego Garay-Ruiz, Mireia Segado-Centellas, Carles Bo
	Title: Predicció de l'especiació aquosa de heteropolioxometalats: el fosfomolibdat i l'arsenomolibdat.
	Type of Contribution: Flash communication
	Congresss: 2ª Reunió de Química Inorgànica i Organometàl·lica de la SCQ
	Year: 2025
	Location: Tarragona, Espanya

d) International Research Stays

1	**Academic position:** Pre-doctoral researcher **Institution:** University of Oslo. Hylleraas Centre of Excellence for Quantum Molecular Sciences **Supervisor/s:** Prof. David Balcells Badía **Grant:** FPI (MINCIN)(PRE2021-097195) – Mobility Budget **Dates:** 26 February 2024 to 27 May 2024 (3 months) **Research topic:** Machine Learning algorithms for the prediction of thermodynamical properties of polyoxometalates.

6) Mentoring and supervision

Student	Position	Center	Year (s)
Laura Sussane Junkers	PhD secondment	ICIQ	2024 (3 months)
Farzaneh Hosseini	Phd	ICIQ	Jan 2025 - today

7) Competitive Grants

1	**Grant/Fellowship:** 2021 ICIQ International PhD Fellowship Programme **Funding Institution:** Ministerio de Ciencia e Innovación **Duration:** 9 months **Research institution:** Institute of Chemical Research of Catalonia

2	**Grant/Fellowship:** FPI pre-doctoral grant PRE2021-097195 **Funding Institution:** Ministerio de Ciencia e Innovación **Duration:** 2 years and 5 months **Research institution:** Institute of Chemical Research of Catalonia

3	**Grant/Fellowship:** FPI – Postdoctoral orientation Period (POP) **Funding Institution:** Ministerio de Ciencia e Innovación **Duration:** 5 months

	Research institution: Institute of Chemical Research of Catalonia

8) Participation in projects

1	**Funding Institution:** Ministerio Español de Ciencia, Innovación y Universidades **Project reference:** PID2020-112806RB-I00 **Dates:** 2021-2023 **Principal Investigator:** Prof. Carles Bo Jané

2	**Funding Institution:** Ministerio Español de Ciencia, Innovación y Universidades **Project reference:** PID2023-152244NB-I00 **Dates:** 2024-2026 **Principal Investigator:** Prof. Carles Bo Jané

3	**Funding Institution:** Programa excelencia Severo Ochoa **Project reference:** CEX2019-000925-S **Dates:** 2020-2024 **Principal Investigator: ---**

4	**Funding Institution:** Agència de Gestió d'Ajudes Universitàries i d'Investigació (AGAUR) **Project reference:** PID2020-112806RB-I00 **Dates:** 2022-2025 **Principal Investigator:** Prof. Carles Bo Jané