

Lluís Artus | Dr.

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🌐 <https://lluisartussuarez.github.io/>



Personal Statement

PhD in computational chemistry, specializing in the simulation of catalytic systems. I have been studying CO₂ hydrogenation mechanisms for seven years and enantioselective hydrogenation of olefins for two years. Using density functional theory, classical molecular dynamics, and microkinetic modeling, I can study the role of catalysts in the reactions. That information is essential to identify favorable and detrimental factors that determine the reaction rates and allow the development of faster and more stable catalysts.

Machine learning applied to theoretical chemistry is rising in popularity. Therefore, last year, I started training myself in it. I have been reading about state-of-the-art ML techniques, attending an ML conference applied to computational chemistry, and, in November 2023, enrolling in IBM's online course on Machine Learning. There, I learned about exploratory data analysis, regression, classification, and unsupervised models, but it will also cover genetic models and deep learning. I look forward to implementing what I learned into a practical application.

Professional experience

Science.....

KTH Royal Institute of Technology	Stockholm, Sweden
Postdoctoral researcher	2022-2024
Project: "Forcefields for electrochemistry in metal-organic frameworks"	
Project: "Reaction mechanisms of enantioselective hydrogenation of olefines"	

Nordic Consortium for CO₂ Conversion	Scandinavia
Postdoctoral researcher	2022-2024
Project: "Modelling of CO ₂ electroreduction in metal-organic frameworks"	
PhD student	2018-2021
Project: "Rational catalyst design for the hydrogenation of CO ₂ derivatives"	

Lecturer in.....

Workshop in Microkinetic Modeling with COPASI	2022
Stockholm, Sweden. April 28-29	
Workshop in Microkinetic Modeling with COPASI	2019
Tromsø, Norway. March 26-27	

Internships.....

Iceland University, Iceland	2022
Group of Egill Skúlason. Ab-initio molecular dynamics. November	

Valladolid University, Spain	2018
Group of Martin Jaraiz. Microkinetic modelling. June – July	
ICIQ, Spain	2015-2016
Group of Feliu Maseras. Modelling of single electron transfers.	
GMMF, Spain (Not paid)	2014-2015
Group of E. Carolina Sañudo. Synthesis and characterization of magnetic and fluorescent molecules.	
Others	
Frenchie Bistro	Oslo, Norway
Waiter	Sept. 2021 – Feb. 2022
Skogstad Hotel ***	Hemsedal, Norway
Waiter and housekeeper	Summer. 2021
Hotel Port-Bó****	Palafrugell, Spain
Receptionist	Summers 2013 – 2015
Hotel & Spa Mas de Torrent *****	Torrent, Spain
Receptionist	Summers 2009 – 2010

Education

Academic education	
Oslo University	Oslo, Norway
Ph.D. Chemistry	2016-2021
Thesis: "Computational study on the deaminative hydrogenation of amides catalyzed by base metal complexes"	
Rovira i Virgili University	Tarragona, Spain
M.Sc. Chemistry	2015-2016
Thesis: "Computational characterization of the mechanism of the reaction between Fe(I) complexes and aryl halides"	
Barcelona University	Barcelona, Spain
B.Sc. Chemistry	2010-2015
Thesis: "Synthesis and characterization of coordination compounds with a fluorescent ligand"	

Courses and Certifications	
Unsupervised Machine Learning	2024
Online. IBM course of >23h. June	
Supervised Machine Learning: Classification	2024
Online. IBM course of >24h. April	
Singularity workshop	2024
Stockholm, Sweden. February 12	
Supervised Machine Learning: Regression	2024
Online. IBM course of >20h. February	
Exploratory Data Analysis for Machine Learning	2023
Online. IBM course of >14h. December	
Introduction to GPUs course	2023
Stockholm, Sweden. October 12-13	

Alpha fold v2.0 and RoseTTAFold Workshop

2021

Online. Aug. 31-Sep. 1

8th MOLCAS Users' Workshop

2017

Uppsala, Sweden. Nov. 20-24

Skillset

Computational chemistry

Reaction mechanism exploration

Software: Gaussian, Jaguar (Schrodinger), COPASI, Acuchem

Rational catalyst design of organometallic catalysts.

Microkinetic modelling for the design and interpretation of experimental kinetic experiments and for the evaluation of theoretical models.

Drug discovery and material science

Software: Amber, Gromacs, CP2K

Forcefield parametrization of organometallic systems

Free energy calculations: FEP, EVB, umbrella sampling, metadynamics

Properties calculations: binding energies, diffusion coefficients, viscosities...

Cheminformatics

Software: RDKit, OpenBabel, molSimplify

Automatic interpretation of chemical databases

Automatic generation of molecular structures for future processing (e.g. machine learning)

Others

Software: NBO6, NCIPLOT, OpenMolcas, Chemcraft, PHI, ioChem-BD

Experimental chemistry

Basic training in

Good laboratory practices, NMR, MS, UV-Vis, FT-IR, Spectrofluorometry, HPLC, GC and SQUID.

Informatics

I have worked with supercomputers and computer clusters for eight years, at a user level.

I am comfortable with python, and have basic knowledge of C++, Fortran, bash, awk and seq.

The python libraries I use most are os, sys, shutil, pandas, numpy, scipy, matplotlib, seaborn, sklearn, rdkit, molSimplify and OpenBabel.

Most of my programming has been scripting for workflow automation or data analysis.

I have recently started studying machine learning. So far, I have completed IBM online courses on "Exploratory Data Analysis" and "Machine Learning regression models".

Publications

Seven articles published in scientific journals. H index of five. Cited more than a hundred times. Five first-authorships.