Lluis Artus | Dr.

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Personal Statement

PhD in computational chemistry, specializing in the simulation of catalytic systems. I have been studying CO_2 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 CO_2 Conversion — Scandinavia
Postdoctoral researcher — 2022-2024
Project: "Modelling of CO2 electroreduction in metal-organic frameworks"

PhD student — 2018-2021
Project: "Rational catalyst design for the hydrogenation of CO_2 derivates"

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.