Yaidel Toledo González

Researcher with vast experience in Computational Simulations with DFT, MD, and coding

Email	yaidel.ovn32@aleeas.com
Web Page	yaidel.poview.org
Instutution	IPREM, University of Pau and the Adour Countries, France

Who I am

With more than 6 years of experience as a Scientific Researcher, I have conducted at least 4 research projects by now, and 2 of them included high loads of coding in either FORTARN, C++, or Python. However, using Python libraries to perform small simulations, data analysis, and representations has always been a day-to-day task.

At the University of Havana we building from scratch a Molecular Dynamics code in FORTRAN to simulate the Matrix Isolation deposition process of impurities into rare gases matrices, under the supervision of Prof. German Rojas Lorenzo. Afterwards, my abilities in physical-chemistry were employed to investigate the reaction mechanism, and provide insights into the atomic processes, characterizing the performance of urea-based foldamers as catalysts, at the University of Pau, under the supervision of Prof. Philippe Carbonniere and Prof. Jean-Marc Sotiropoulos. Then, with my expertise using Computational Simulations software, we delve into the use of Ruthenium complexes as catalysts to storage and release H_2 using CO_2, still at the Univ. of Pau.

I love managing projects, either professional or personal, photography, coding, web design, writing, baseball, calisthenics, and gardening. If you would like to know more about me, do not hesitate to send me an email.

> I have faith in human betterment, in the future life, in the usefulness of virtue, (...)
>
> José Martí, 1882

Areas of expertise

Quantum Chemistry software	Gaussian, deMon2k, Multiwfn
Programming languages	Fortran, Python, C/C++
Data Analysis	Python libraries: pd, mpl, numpy, etc
Linux OS related skills	Linux, Bash, Emacs, Git, LaTeX
High Performance Computing	HPC at TGCC Juliot-Curie
Research Project Management	Writing Proposal, Project Management
Engineering	AutoCAD, Ansys: FEA, and CFD

Work Experience

Researcher, Post-doc **2023 – 2024**

IPREM, University of Pau and the Adour Countries, France

I carried our computational simulations to provide insights into the hidden processes at the atomic scale in Ru based catalysts to storage H_2 and CO_2 into formic acid, and then release them. — The project title was "Chemical storage of Hydrogen by homogeneous catalysis using Ruthenium complexes: a DFT approach", and it was financed by ISIFoR (Institut Carnot). Under the supervision of Prof. P. Carbonniere and J.M. Sotiropoulos.

Researcher, Ph.D. student **2019 – 2022**

IPREM, University of Pau and the Adour Countries, France

I performed computational simulations (DFT, SE-PM6, MD, ONIOM), coding with Bash and Python, data analysis, research, etc., to identify the reaction mechanisms defining the catalytic properties of urea-based foldamers to achieve challenging C-C bond forming reactions. This work promises to have great impact on pharmaceutical and agricultural applications. — The project title was "Molecular design for catalytic activities of helical chiral oligoureas", and it was financed by the ANR. Ph.D obtained as result on December 2022. Under the supervision of Prof. P. Carbonniere and J.M. Sotiropoulos.

Researcher, student **2018 – 2019**

InsTEC, Univerity of Havana, Cuba

We build a Molecular Dynamics code from scratch using FORTRAN, specifically tailored to simulate the Matrix Isolation processes of impurities in rare gases matrices. — The project title was "Study of confinement, relaxation and energy transfer processes of atomic and molecular systems", and it wasfFinanced by the National Basic Sciences Program. Degree in Engineering in Nuclear and Energy Technologies obtained as result on June 2019. Under the supervision of Prof. Germán Rojas Lorenzo.

Researcher, student **2015 – 2018**

InsTEC, Univerity of Havana, Cuba

Employing Molecular Dynamics we were able to simulate the interaction of small molecules with environmental interest in an idealized situations. — The project title was "Physical-chemical study of atomic and molecular systems with interest for the environment", financed by InsTEC. Under the supervision of Prof. Germán Rojas Lorenzo.

Languages

Spanish	Native	●●●●●
English	C1	●●●●○
French	B2	●●●○○

Education

Ph.D. degree in Physical-Chemistry — 2022

IPREM, University of Pau and the Adour Countries, France

"Molecular design for catalytic activities of helical chiral oligoureas." Under the supervision of Philippe Carbonniere, and Jean-Marc Sotiropoulos.

Engineer in Nuclear and Energetic Facilities — 2019

InsTEC, Univerity of Havana, Cuba

"Matrix isolation of $W(CO)_6$: understanding at the atomic scale of the materials design." *Cum Laude*. Under the supervision of Germán Rojas Lorenzo.

Training and Workshops

IAEA Internet Reactor Laboratory - IRL — 2018

At the RA-6 research reactor of the National Atomic Energy Commission (CNEA) at the Centro Atómico Bariloche (CAB), in Argentina

Six laboratory sessions between 11/09/2018 and 20/11/2018, detailing the functioning and management of the experimental reactor with full access to the Control Room.

Molecular Dynamics Fundamentals — 2017

Institute of Materials Sciences and Tecnologies, University of Havana, Cuba

Training in the frame of the XXIV International Summer School in Materials Sciences and Technologies, between 20/11/2017 and 01/12/2017.

Specific skills

R&D ●●●●○	deMon2k ●●●○○	Molecular Dynamics ●●●○○
Sci. Writing ●●●○○	MultiWFN ●●●○○	HPC ●●●○○
Project Management ●●○○○	ANSYS ●●●○○	Coding ●●●●○
Numerical Simulations ●●●●○	AutoCAD ●●●○○	Python/FORTRAN ●●●●○
Gaussian ●●●●○	DFT ●●●●○	C/C++ ●●●○○

Git ●●●●○	Linux ●●●●●	Emacs ●●●●○
Bash ●●●●○	LaTeX ●●●●○	Office suite ●●●●●

Publications

[1] Yaidel Toledo-González, Faykat Ahmed, Jean-Marc Sotiropoulos, et al. "Evaluation of the Donor Character for Urea-Based Foldamers throughout the Empirical Estimation of pKa". *Theoretical Chemistry Accounts* 142.8 (Aug. 2023), p. 67.

[2] Yaidel Toledo-González. "Molecular Design for Catalytic Activities of Helical Chiral Oligoureas". PhD thesis. Pau, France: University of Pau and the Adour Countries, Dec. 7, 2022.

[3] Yaidel Toledo-González, Jean-Marc Sotiropoulos, Diane Bécart, et al. "Insight into Substrate Recognition by Urea-Based Helical Foldamer Catalysts Using a DFT Global Optimization Approach". *The Journal of Organic Chemistry* 87.16 (Aug. 19, 2022), pp. 10726–10735.

[4] Daniel Camacho-Granados, Yaidel Toledo-González, Miguel Lara-Moreno, et al. "A Simulation of Tungsten Hexacarbonyl Matrix Isolation". *Revista Cubana de Física* 37.1 (2020).

Research grants and fellowships

Computation time grant of 1M CPU/hours **2023**

🏛 *Granted by GENCI, at TGCC*

☑ *Project*: "Chemical storage of Hydrogen by homogeneous catalysis: modelation and dynamics of the systems properties"

Computation time grant of 450k CPU/hours **2023**

🏛 *Granted by GENCI, at TGCC*

☑ *Project*: "Hydrophosphination of alkynes directed by hydrogen bonds"

Computation time grant of 900k CPU/hours **2021**

🏛 *Granted by GENCI, at TGCC*

☑ *Project*: "Modélisation moléculaire pour l'étude des propriétés catalytiques de foldamères hélicoïdaux à base d'urée"

Seminars and Conferences

Oral Communication **02/2024**

Journées Grand Sud-Ouest de la Société Chimique de France (SCF-GSO2024), Bordeaux, France

Urea-based foldamer catalyst for C-C bond forming in asymmetric Michael reaction: a DFT investigation

Oral Communication **09/2023**

COTAW XII, Namur, Belgium

Base-free reversible hydrogen storage using a tethered η^5-Oxocyclohexadienyl Ruthenium Complex: a DFT investigation

Oral Communication **09/2023**

Munich Foldamers 2023 Symposium, Munich, Germany

Urea-based foldamer catalyst for C-C bond forming in asymmetric Michael reaction

Oral Communication **07/2022**

International Conference on Noncovalent Interactions (2ICNI), Strasbourg, France

Molecular recognition for C-C bond forming in asymmetric Michael reaction with urea-based foldamer catalyst: Molecular modelling from DFT global optimization

Poster **06/2022**

12th Congress on Electronic Structure: Principles and Applications (ESPA2022), Vigo, Spain

Molecular design for catalytic activities of helical chiral oligoureas

Seminar Talk **06/2022**

Pôle CAPT Seminar at the IPREM, Univ. Pau, Pau, France

Urea-based oligomers as efficient catalysts: a DFT Global Optimization approach

Oral Communication **09/2021**

Rencontres de Physique-Chimie 2021 (RCP 21), Sète, France

Molecular design for catalytic activities of helical chiral oligoureas

Poster **01/2021**

Midlands Computational Chemistry Meeting, Virtual Conference

Molecular design for catalytic activities of helical chiral oligoureas

Oral Communication **11/2020**

Journées "Théorie, Modélisation et Simulations" (*JTMS2020*), *Virtual Conference*

Molecular design for catalytic activities of helical chiral oligoureas

Poster **06/2019**

12th Seminars of Advanced Studies on Molecular Design and Bioinformatics (*SEADIM*), *Cayo Santa María, Cuba*

Molecular Dynamics simulation of a deposition model for CuO deposition on Al

Oral Communication **2019**

Student Scientific Forum "InSTEC 2018-2019", Havana, Cuba

$\mathrm{W(CO)_6}$ matrix isolation: understanding of the atomic scale in the design of materials

Oral Communication **2018**

Student Scientific Forum "InSTEC 2017-2018", Havana, Cuba

Classical Molecular Dynamics simulation of Al/CuO deposition

Oral Communication **2017**

Student Scientific Forum "InSTEC 2016-2017", Havana, Cuba

Migration to the LaTeX platform of Quantum Physic conferences

Teaching experience

Laboratory of Electromagnetism **2018**

InsTEC, University of Havana

72 hours. Were given in Spanish language.

Laboratory of Optics **2018**

InsTEC, University of Havana

48 hours. Were given in Spanish language.

Supervised students

Faykat Ahmed **2021**

Université de Pau - Université Gustave Eiffel - Université Paris-Est Créteil

Master 2 PCMA: Evaluation of the donor character for urea-based foldamers throughout the empirical estimation of their $\mathrm{pK_a}$.

Daniel Camacho Granados **2019**

InsTEC, University of Havana

BSc: Matrix isolation of $\mathrm{W(CO)_6}$ in Neon matrices using Molecular Dynamics

Awards

First place **2019**

Commission of Theoretical and Experimental Physics in the Student Scientific Forum "InSTEC 2018-2019", Havana, Cuba

For the Oral Communication "$\mathrm{W(CO)_6}$ matrix isolation: understanding of the atomic scale in the design of materials"

Third place **2018**

Commission of Theoretical and Experimental Physics in the Student Scientific Forum "InSTEC 2017-2018", Havana, Cuba

For the Oral Communication "Classical Molecular Dynamics simulation of Al/CuO deposition"

Third place **2017**

Contest ACM-International Collegiate Programming Contest (ACM-ICPC) Final InSTEC 2017, Havana, Cuba

Team `randname`

Third place **2016**

Contest ACM-International Collegiate Programming Contest (ACM-ICPC) Final InSTEC 2016, Havana, Cuba

Team `instec++`