Muammar W. El Khatib Rodriguez, Ph.D.

EDUCATION

Ph.D. in Theoretical Chemical Physics July 2012 to July 2015.
Université Paul Sabatier III, Toulouse, France.
Thesis title: "Characterization of metallic and insulating properties of low-dimensional systems."
I was awarded with funding from L'Agence Nationale de la Recherche to work in a bilateral project between France and Germany.
Supervisors: Prof. Stefano Evangelisti, and Prof. Thierry Leininger.
Laboratory: Laboratoire de Chimie et Physique Quantiques.
Group: Méthodes et outils de la Chimie Quantique.

Master on Theoretical Chemistry and Computational Modelling September 2010 to July 2012.
Université Paul Sabatier III, Toulouse, France.
Thesis title: "An *ab initio* potential energy surface for quantum reactive scattering calculations."
I was awarded with an Erasmus Mundus Scholarship to do my studies in different European universities.

Bachelor of Science, Chemistry May 2010.
Universidad del Zulia, Maracaibo, Venezuela.
Thesis title: "Determination of the linear and nonlinear optical properties of the nitrogenous bases of DNA, RNA and their respective tautomers".

Technician in Computer Repair and Troubleshooting 2003.
Instituto Los Próceres, Maracaibo, Venezuela.

Secondary Education, Bachelor of Science 2000.
Colegio San Vicente de Paúl, Maracaibo, Venezuela.

LANGUAGES

Spanish, Native language.
English, Full professional proficiency.
French, Full professional proficiency.

SCIENTIFIC WORK EXPERIENCE

Bristol Myers-Squibb November 2020 to present.
Informatics and Predictive Sciences organization. (Principal Machine Learning Scientist)
200 Cambridge Park Drive, Cambridge, MA 02140, USA.

This role will provide collaborative, creative, and interdisciplinary applied machine learning research in partnership between Informatics Predictive Sciences (IPS) and Chemistry organizations.

- Reporting to the lead for Predictive Drug Substance Research, scenarios will involve a range of datasets and learning objectives, including for example drug discovery, structural biology, multi-modal modeling and prediction for chemical and biological datasets.
- Formulation and implementation of predictive modeling and machine learning solutions for the optimization of chemical structures and properties.
- Application of cutting-edge machine learning (deep learning) approaches to structural biology and molecular interaction challenges.
- Design and generation of integrated chemical and biological data assets for predictive research in partnership with internal and external collaborators. The successful candidate will work alongside experts in familiar applications of machine learning in the biotechnology domain, including:
    1. Collaboration to develop human-in-the-loop systems to capture and operationalize machine learning datasets and algorithms used by BMS scientists.
    2. Application of supervised, self-supervised, semi-supervised deep learning methods to derive robust generalizable and reusable representations for chemical and biological assay data.
    3. Design of multi-task, multi-modal and generative neural network learning approaches to tackle real-world drug discovery optimization problems, including prediction of both assayed and abstract compound properties.
    4. Contribution to design and development of Machine Learning data repositories focused on proteins and chemical compounds.
- Pursue leading research in applied machine learning that demonstrates the value of predictive methods to accelerate and optimize drug development.
- Derive and apply predictive approaches in collaboration with BMS colleagues in the Informatics and Predictive Sciences, and Chemistry departments.
- Apply rigorous internal standards for applied machine learning practice, including evaluation of methods, approaches and solutions.
- Contribute to broader data analysis and predictive methods strategies across the business as required, including assessment of 3rd party capabilities.
- Present strategies, approaches, results and conclusions to BMS colleagues and external audiences.
- Contribute to enable strategic collaborations with academic and commercial collaborators to benefit therapeutic programs.

Lawrence Berkeley National Laboratory November 2018 to September 2020.
Computational Research Division. (Postdoctoral Scholar in Machine Learning and Chemical Sciences)
1 Cyclotron Road, MS 50F-1650 Berkeley, CA 94720, USA.

- Developed a python library to ease the deployment of machine learning models for chemistry and materials sciences. `https://github.com/muammar/ml4chem`. This package is helping us advance our research faster because we can consistently implement new methods.
- Developed a neural network model that can learn how to predict retention times from chromatography data. These models can be used by experimentalists to get insights about the substances they study without explicitly running the experiments.
- Applied autoencoders to extract features and systematically studied their topology to understand their effect on the predictive power of models used for material sciences.

- Generated data sets using web-scraping and diversified their variance with active learning techniques.
- Worked on a project for Scaling Interactive Science for Data-Intensive Discovery for the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory.
- Led and designed research projects executed by summer interns.
- Wrote scientific publications to show our results to the community.

Brown University October 2016 to November 2018.
School of Engineering. (Postdoctoral Research Associate)
Box D. Brown University. 184 Hope Street. Providence, RI 02912 USA.

- Worked on the acceleration of electronic structure calculations using machine learning models to decrease orders of magnitude the computational time needed by the simulations.
- Was actively involved in the development of the Atomistic Machine-learning Package (Amp) created and maintained by the Catalyst Design laboratory at Brown University `https://bitbucket.org/andrewpeterson/amp`.
- Implemented kernel ridge regression within an atom-centered mode in their machine learning package.
- Participated in the design of scientific projects and supervision of students during their research in our laboratory.
- Presented scientific results in international conferences.

Laboratoire de Chimie et Physique Quantiques April 2011 to July 2015.
Université Paul Sabatier III. Toulouse, Occitanie, France. 31000. (Master and Ph.D. Candidate)

- **Master Student: April 2011 to June 2012**
  - Internship: Studied the electronic and magnetic properties of polyacenes of finite sizes using post-Hartree-Fock Methods (CASSCF and NEVPT2), and the suite of programs provided in the MOLPRO package. This work was part of a required internship to fulfill the first year of the European Master on Theoretical Chemistry and Computational Modelling under the supervision of Prof. Stefano Evangelisti, and Prof. Thierry Leininger.
- **Ph.D. Candidate: July 2012 to July 2015**
  - Ph.D. Thesis: "Characterization of metallic and insulating properties of low-dimensional systems."
  - Implemented the Position Spread Tensor (TPS) in the complete active space self-consistent field (CASSCF) module of the MOLPRO package.
  - Production of scientific publication and presentation of results in international conferences.

Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie October to November 2013.
(Guest Scientist)
Freie Universität Berlin.
Takustraße 3. 14195 Berlin, Brandenburg, Germany.

- Investigated polyacenes of different shapes using the method of the increments at *ab initio* level.

Gruppo di Dinamica dei Processi Chimici Elementari February 2012 to May 2012.
Università degli Studi di Perugia. (Master Student)
Via Elce di Sotto, 8, 06123. Perugia, Umbria, Italy.

- Quantum scattering study of a collision reaction between a diatomic molecule and a proton. We performed the construction of the potential energy surfaces at multi-reference configuration interaction level using the MOLPRO package.
- This work was part of my Master's Degree Thesis under the supervision of Prof. Antonio Laganà and Ph.D. Leonardo Pacifici.

Laboratorio de Química Inorgánica Teórica (LQIT) April 2004 to May 2010.
La Universidad del Zulia, Maracaibo, Zulia, Venezuela. (Research Assistant)

- Carried out a dissertation in the area of Quantum Chemistry calculating the Optical Response of materials using density functional theory (DFT).
- Thesis: "Determination of the Linear and Nonlinear Optical Properties of the Nitrogen Basis of DNA, RNA and Their Tautomers."
  Supervisor: Prof. Humberto Soscún.
- Volunteer and maintainer of the computers in the Laboratory.

Laboratory of Computational Catalysis of PDVSA - Intevep May 2008 to August 2008.
R&D of HDHPLUS® and RIRP. (Intern)
PDVSA-Intevep, S.A. Los Teques, Miranda.
Postal Code: 76343.
Caracas 1070A, Venezuela.
Phones: +58 (0) 212 33 06 011 - fax: +58 (0) 212 33 06 448

- A theoretical study of asphaltenes from Kuwait oil refineries was carried out by using semi-empirical and density functional theory methods. Their composition was similar to those asphaltenes precipitating in Venezuelan oil refineries in Merey, Merey - Mesa and Zuata refineries. We characterized, modeled and optimized them to understand their chemical physical properties.

TEACHING EXPERIENCE

Département de Physique January 2013 to June 2015.
Faculté des Sciences et de l'Ingénierie (Teaching Assistant)
Université Paul Sabatier III. 31000. Toulouse, Occitanie, France.

Courses

- "Physique 1 et outils informatiques (EDST2BCM)".
  - Geometrical Optics.
  - Focométrie (measure of focal distances).
  - Fluid mechanics.
  - Capillarity.
- "Physique 2 (EDST1ABM): Prolongement de l'enseignement de physique de terminale S avec approfondissement et acquis des bases de modélisation de diférents phénomènes sous forme de thèmes":
  - Basic notions of electricity.
  - Kinematics, Newton's laws, and ballistics.
  - Harmonic and damped oscillators.
  - Circular movement.
  - Energy and electrical power.

IT EXPERIENCE

Debian Project May 2006 to present.
`http://www.debian.org`

- Debian Developer (muammar@debian.org). For a list of packages maintained by me please visit:
  `http://qa.debian.org/developer.php?login=muammar`

Github Projects present.

- For a list of developed software, my portfolio is available at `https://github.com/muammar/`.

SEGECOM Zulia May 2009 to June 2010.
3H Avenue, Salto Angel Mall, Office 1. Maracaibo, Zulia, Venezuela. (System Administrator)

- System and network administrator.
- Configuration of maintenance gateway server using Astaro Firewall.
- Quality assurance of the following services: Apache2 web server, Mysql database server, Samba server, and FTP server.
- Free software consultant for SEGECOM branch in Caracas, Venezuela.

Cooperative Association. GEEKCORP October 2008 to July 2009.
Las Margaritas Street, La Asunción. Nueva Esparta.
Margarita Island, Venezuela. (Software Developer)

- Free software consultant and software developer in the area of packaging for Debian specific Linux Distributions. We developed a modified Linux distribution based on Debian GNU/Linux for the Venezuelan government.

PEER REVIEW ACTIVITIES

1. Nature: npj Computational Materials.
2. American Institute of Physics (AIP): The Journal of Chemical Physics.
3. ScienceDirect: Catalysis Today.
4. Taylor & Francis: Molecular Simulation.

LIST OF PUBLICATIONS

My Google Scholar Page
`https://scholar.google.com/citations?user=WBXXCScAAAAJ&hl=en`.

1. **M. El Khatib**, S. Evangelisti, T. Leininger, G.L. Bendazzoli, "A Theoretical Study of Closed Polyacene Structures", *Phys. Chem. Chem. Phys.*, 14, 15666 (2012).
   DOI: 10.1039/C2CP42144E.
2. O. Brea, **M. El Khatib**, C. Angeli, G.L. Bendazzoli, S. Evangelisti, T. Leininger, "Behavior of the Position-Spread Tensor in Diatomic Systems", *J. Chem. Theory Comput.*, *9*, 5286 (2013).
   DOI:10.1021/ct400453b
3. **M. El Khatib**, T. Leininger, G.L. Bendazzoli, S. Evangelisti., "Computing the Position-Spread tensor in the CAS-SCF formalism", *Chem. Phys. Lett.*, 591, 58 (2014).
   DOI:10.1016/j.cplett.2013.10.080.
4. G.L. Bendazzoli, **M. El Khatib**, S. Evangelisti, T. Leininger, "The Position Spread Tensor in Mixed-Valence Compounds: a Study on the H_4^+ Model System", *J. Comput. Chem.*, 35, 802 (2014). (Cover image is shown below).
   DOI: 10.1002/jcc.23557
5. **M. El Khatib**, S. Evangelisti, T. Leininger, G.L. Bendazzoli, "Partly Saturated Polyacene Structures: a Theoretical Study", J. Mol. Model. 20, 2284 (2014).
   DOI: 10.1007/s00894-014-2284-7
6. **M. El Khatib**, G. L. Bendazzoli, S. Evangelisti, W. Helal, T. Leininger, L. Tenti, C. Angeli, "Beryllium-Dimer: a Bond based on non-Dynamical Correlation", J. Phys. Chem. A, 6664 (2014).
   DOI: 10.1021/jp503145u.

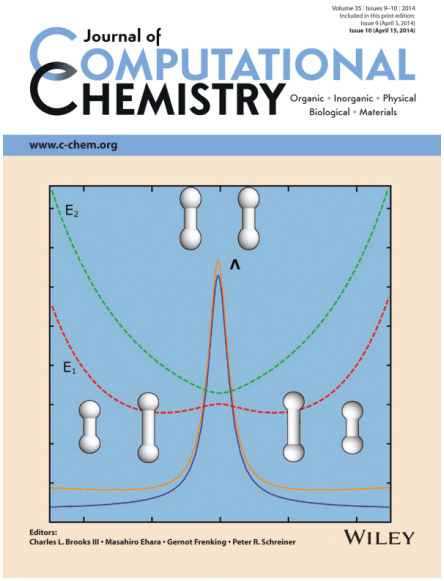

Figure 1: The $(H_2{-}H_2)^+$ system exhibits a mixed-valence character when the two hydrogen dimers are sufficiently apart, with the hole localized on the dimer with the longest bond. The cover shows energies of the two lowest electronic states (dashed lines) as a function of a reaction coordinate ξ that connects the two ground-state minima. On page 802, Gian Luigi Bendazzoli et al. find that the total position-spread tensor Λ is a powerful indicator of the electron delocalization within the two molecules. A spectacular peak of Λ is found for both the ground and the excited states in the transition state region.

7. **M. El Khatib**, O. Brea, E. Fertitta, G.L. Bendazzoli, S. Evangelisti, T. Leininger, B. Paulus, " Spin delocalization in hydrogen chains described with the spin-partitioned Total-Position Spread tensor", Theor. Chem. Acc., 134, 1 (2015).
   DOI: 10.1007/s00214-015-1625-7
8. **M. El Khatib**, O. Brea, E. Fertitta, S. Evangelisti, T. Leininger, G.L. Bendazzoli, "The total position-spread tensor: spin partition", J. Chem. Phys. 142, 094113 (2015).
   DOI: 10.1063/1.4913734
9. E. Fertitta, **M. El Khatib**, G.L. Bendazzoli, S. Evangelisti, T. Leininger, B. Paulus, "The Spin-Partitioned Total-Position Spread tensor: an application to Heisenberg spin chains", J. Chem. Phys., 143, 244308 (2015).
   DOI: 10.1063/1.4936585
10. O. Brea, **M. El Khatib**, C. Angeli, G.L. Bendazzoli, S. Evangelisti, T. Leininger, "The Spin-Partitioned Total-Position Spread: an application to diatomic molecules", J. Phys. Chem. A, 120, 5230 (2016).
    DOI: 10.1021/acs.jpca.6b01043
11. A. Khorshidi, Z. Ulissi, **M. El Khatib**, A.A. Peterson, Amp: The Atomistic Machine-learning Package v0.5, (2017).
    DOI: doi:10.5281/zenodo.322427
12. A. Khorshidi, **M. El Khatib**, A.A. Peterson, Amp: The Atomistic Machine-learning Package v0.6, (2017).
    DOI: doi:10.5281/zenodo.836788
13. **M. El Khatib**, "ML4Chem: A Machine Learning Package for Chemistry and Materials Science", arXiv (2020).
    DOI: arXiv:2003.13388.
14. M.D. Hanwell, WA. De Jong, J. Hachmann, C. Harris, A. Genova, **M. El Khatib**, P. Avery, "Open Chemistry, JupyterLab, REST, and Quantum Chemistry" Int J Quantum Chem (2020); e26472.
    DOI: 10.1002/qua.26472
15. Y.H. Tang, **M. El Khatib**, W.A. de Jong, "Uncertainty Quantification and Outlier Detection on Noisy Data" in preparation.
16. **M. El Khatib**, W.A. de Jong, "Extraction of Atomic Features using Autoencoders" in preparation.

PRESENTATIONS, PROCEEDINGS & SEMINARS

Scientific

- Oral presentation: 'Feature Extraction Using Semi-Supervised Deep Learning.", in the APS 2020 March Meeting. 2^{nd} to 6^{th} March 2020. Denver, CO, United States.
- Oral presentation: "ML4Chem: a framework to facilitate machine learning for chemistry and materials science", in the 2019 Data Science Institute Workshop of Lawrence Livermore National Laboratory. 23^{rd} to 24^{th} July 2019. Garre Vineyard & Winery 7986 Tesla Road Livermore, CA, United States.
- Discussion Leader for the "Ab Initio and Data-Driven Modeling" session of the Gordon Research Seminar, and Poster presentation: "Local Chemical Environments In Machine Learning" in the Gordon Research Conference: *Towards Next-Generation Challenges in Computational Chemistry: From Quantum Chemistry and Molecular Simulation to Data Discovery and Quantum Computing.* 21^{st} to 27^{th} July, 2018. West Dover, VT, United States.
- Oral presentation: "Acceleration of Saddle-Point Searches Assisted by Machine Learning". The 68^{th} Annual Meeting of the International Society of Electro-chemistry. 31^{st} August, 2017. Providence, RI, United States.
- Member of the organizing committee, teacher and web master of the TCCM Winter School *Tutorials in Theoretical Chemistry* organized by the Université Paul Sabatier in February 2016. Saint-Lary-Soulan, France. `http://www.irsamc.ups-tlse.fr/lttc/`.
- Member of the organizing committee, teacher and web master of the TCCM Winter School *Tutorials in Theoretical Chemistry* organized by the Université Paul Sabatier in February 2015. Luchon Superbagnères, France. `http://www.irsamc.ups-tlse.fr/lttc/2015`.
- Poster presentation: "Total Position Spread tensor in mixed-valence systems: an indicator of charge transfer processes" in the *50^{th} Symposium on Theoretical Chemistry 2014 (STC 2014)* held from 14^{th} to 18^{th} September, 2014. Vienna, Austria.
- Member of the organizing committee, and web master of the *9th edition* of the Intensive Course of the European Master in Theoretical Chemistry and Computational Modelling (TCCM) held at the Université Paul Sabatier in September 2014. Toulouse, France. `http://www.irsamc.ups-tlse.fr/tccm2014/`.
- Oral communication: "Metal-insulator transition in low-dimensional systems". Poster presentation: "Total Position Spread tensor in mixed-valence systems: an indicator of charge transfer processes" in the *9th Congress on Electronic Structure: Principles and Applications (ESPA)* held from 1^{st} to 4^{th} July, 2014. Badajoz, Spain.
- Seminar in the group of Prof. Beate Paulus during my scientific visit to her group. Oral communication: "On the total position spread tensor in some model systems" held on 22^{nd} October 2013 in the Freie Universität Berlin. Takustraße 3. 14195 Berlin, Germany.
- Poster presentation: "The behavior of the Position-Spread Tensor in Diatomic Systems" in the *9th edition of the European Conference of Computational Chemistry* held from 1^{st} to 5^{th} September, 2013. Sopron, Hungary.
- Poster presentation: "The behavior of the Position-Spread Tensor in Diatomic Systems" in the *NEXT DAYS* of "Le projet Nano, mesures Extrêmes & Théorie (NEXT)" held from 6^{th} to 7^{th} June, 2013. Le Barcarès, France.
- Poster presentation: "The behavior of the Position-Spread Tensor in Diatomic Systems" in the 7^{th} Molecular Quantum Mechanics (MQM) congress held from the 2^{nd} to the 7^{th} June, 2013. Lugano, Switzerland.
- Attendee to the "Theoretical Chemistry For Periodic Systems: Systematically Improvable Electronic Structure Methods (SIMPS 2013)" held from the 11^{th} to the 15^{th} February, 2013. Ax-les-Thermes, France.

- Poster presentation:"A Theoretical Study of Closed Polyacene Structures" in the *48th Symposium on Theoretical Chemistry (STC 2012)* held from the 23rd to the 27th September, 2012. Karlsruhe Institut für Technologie. Institut für Physikalische Chemie. Abteilung für Theoretische Chemie. Karlsruhe, Germany.
- Poster presentation:"A Theoretical Study of Closed Polyacene Structures" in the *8th Congress on Electronic Structure: Principles and Applications (ESPA)* held from the 2th to 29th June, 2012. University of Barcelona. Barcelona, Spain.
- Poster presentation:"On the electronic structure of cyclic oligocenes" in *The World Association of Theoretical and Computational Chemists (WATOC 2011)*, Santiago de Compostela, Spain 2011.
- Poster presentation: "Determinación de las Propiedades Ópticas Lineales y No Lineales de las Bases Nitrogenadas del ADN, ARN y sus Respectivos Tautómeros" (Determination of the Linear and Nonlinear Optical Properties of the Nitrogen Basis of DNA, RNA and Their Tautomers) to the *"II Congreso de Físico Química Teórica"* (Second Congress of Theoretical Physical Chemistry). Place: Choroní, Aragua. Venezuela. December 2008.
- Aplicación de Software para Científicos y Reacciones ene-retro ene (Application of Scientific Software for Retro-ene Reactions). ENEC. Facultad Experimental de Ciencias. La Universidad del Zulia. Maracaibo, Zulia, Venezuela. 2006.
- Attendee of the *"XXXI Congreso de Químicos Teóricos de Expresión Latina"* (Congress of Theoretical Chemists). QUITEL 2005. Altagracia. Nueva Esparta, Venezuela. October 2005.

IT and Others

- Attendee as Developer to the 8th International Conference of Debian Developers (Debconf). Place: Mar del Plata, Argentina. August 2008.
- Invited speaker: "Terceras Jornadas Regionales de Conocimiento Libre" (Third Regional Congress of Free Software). Place: Universidad de Oriente. Margarita Island, Nueva Esparta. Venezuela. December 2008.
- Invited speaker: "Festival Latino-Americano de Instalación de Software Libre 2008" (Latin American Festival of Free Software Installation of 2008). Place: University Dr. José Gregorio Hernández. Address: 15th Av. Delicias with 89B St. "Facultad de Ingeniería, FING".
- Attendee as Developer, to the 7th International Conference of Debian Developers (Debconf). Place: Teviot Row House (University of Edinburgh). Edinburgh, Scotland. June 2007.
- Invited speaker: "Debian: Comunidad, Desarrollo e Integración". Place: Esquina Avenida Guajira con Circunvalación 2. Universidad Rafael Belloso Chacín (URBE). Maracaibo. Zulia, Venezuela. February 2007.
- Attendee to the "2do Congreso Nacional de Software Libre" (Second National Free Software Congress). Venezuela 2006.
- Invited speaker: "Debian Day Maracaibo". Place: Maracaibo. PDVSA 5 de Julio. Maracaibo. Zulia, Venezuela. August 2006.
- Invited speaker: "4to Foro Mundial de Conocimiento Libre" (Fourth Free Knowledge International Forum). Maturín. Monagas, Venezuela. October 2006.
- Attendee to the "3er Foro Mundial de Conocimiento Libre" (Third Free Knowledge International Forum)
- Attendee to the "X Jornadas Científicas de La Universidad del Zulia". Seminario de las Primeras Olimpiadas Petroleras del CENAMEC (First Oil Olympics Seminar).

COURSES & WORKSHOPS

Scientific

- Machine Learning by Andrew Ng, Online Course at Coursera. 2016.
- Ph.D. Workshop of the European Joint Doctorate Program in Theoretical Chemistry and Computational Modelling. 1^{st} July, 2014. Badajoz, Spain.
- CECAM Theoretical Chemistry and Computational Modelling, Winter School on Large Systems (QCLAMS 2014). Saint-Lary-Soulan, France. January 20^{th}-24^{th}, 2014.
- European Summer School in Quantum Chemistry (ESQC 2013). Torre Normanna, Sicily.
- Ph.D. Workshop of the European Joint Doctorate Program in Theoretical Chemistry and Computational Modelling. Oral communication: "On the total position spread tensor". 5^{th} September, 2013. Sopron, Hungary.
- Ph.D. Workshop of the European Joint Doctorate Program in Theoretical Chemistry and Computational Modelling. Oral communication: "A Theoretical Study of Closed Polyacene Structures". 26^{th} June, 2012. University of Barcelona.
- 6^{th} edition of the International Intensive Course of the European Master in Theoretical Chemistry and Computational Modelling. September 2011. Universitat de València. Valencia, Spain.
- Gaussian Workshop, July 2011. Santiago de Compostela, Spain.
- European School on the Dynamics of Excited States Induced by Ultra Short Pulses. (Zaragoza Scientific Centre for Advanced Modelling, ZCAM). Zaragoza, Spain. 2011.
- Intensive Course: An introduction to Nonlinear Wave Equations. Held in the Physics Department of La Universidad del Zulia, and carried out by Ph.D. David Amundsen from Carleton University, Canada.

IT and Others

- 'C' Language Course. (Universidad del Zulia. Experimental Faculty of Sciences.). Department of Special Programs.
- FORTRAN 90. Language Course. (Universidad del Zulia. Experimental Faculty of Sciences.)
- Study of Classical Guitar. Musical center and academy: "Clavier", Maracaibo, Venezuela.

TECHNICAL SKILLS

- Distributed and parallel computing with the Dask library.
- Pytorch and Scikit-learn machine learning libraries.
- Practical skills using the Pandas data analysis library.
- FireWorks open-source code for defining, managing, and executing workflows in parallel.
- MongoDB databases.
- Skills on writing in the high-quality typesetting system, LaTeX.
- Programming languages: Python, FORTRAN 77, FORTRAN 90,
- BASH scripting.
- Skills on computational quantum mechanical programs such as: GPAW, MOLPRO, Gaussview, Gaussian, Molden, Orca, Jmol, Materials Studio, gOpenMol.
- Skills on the Atomic Simulation Environment (ASE).
- Atomistic Machine Learning Package (Amp).
- Skills on Debian Packaging Programs such as @dh, Debhelper, and CDBS.

- Wide experience in technical service and installation of software in personal computers.
- Basic Knowledge on installation and configuration of networks.
- Practical Knowledge in the use of Microsoft Office, and Libre Office.
- Operating Systems such as: LINUX, in most of its distributions based on Red Hat Package Manager (RPM) and Advanced Package Tool (APT), especially in Debian; Windows; macOS, and basic skills on Free BSD.
- Skills on the compilation and configuration of the Linux Kernel from its source code.
- Skills in the configuration of web servers, FTP servers, SAMBA servers and mail servers (POSTFIX).

INTERESTS

Classical guitar, free software community, physics, machine learning, electronic structure theory, technologies.