

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.

SCIENTIFIC WORK EXPERIENCE

Lawrence Berkeley National Laboratory

November 2018 to present.

Computational Research Division.

(Postdoctoral Scholar)

1 Cyclotron Road, MS 50F-1650 Berkeley, CA 94720, USA.

- My research is related to mass spectra prediction with machine-learning.

Brown University

October 2016 to November 2018.

School of Engineering.

(Postdoctoral Research Associate)

Box D. Brown University. 184 Hope Street. Providence, RI 02912 USA.

- My research is related to the acceleration of electronic structure calculations using machine learning models.
- I am actively involved in the development of the Atomistic Machine-learning Package (Amp) that was created and is maintained in the group of Prof. Andrew A. Peterson <https://bitbucket.org/andrewpeterson/amp>.
- I implemented kernel ridge regression within an atom-centered mode in Amp.
- I participate in the scientific supervision of students during their research in our laboratory.

Laboratoire de Chimie et Physique Quantiques
Université Paul Sabatier III. Toulouse, France. 31000.

April 2011 to July 2015.
(Master and Ph.D. Candidate)

- **Master Student: April 2011 to June 2012**

- Internship: I collaborated doing a theoretical study of 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 carried out as 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.”
- Implementation of the Position Spread Tensor (TPS) in the CASSCF module of the MOLPRO package.

Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie.

October to November 2013.

Freie Universität Berlin.

(Guest Scientist)

Takustraße 3. 14195 Berlin, Germany.

- Polyacenes of different shapes were investigated 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. Via Elce di Sotto, 8, 06123. Perugia, Italy.

(Master Student)

- 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 carried out as 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)

2004 to 2010.

La Universidad del Zulia, Maracaibo, Venezuela.

- I 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

Faculté des Sciences et de l'Ingénierie
Université Paul Sabatier III. 31000. Toulouse, France.

2013 to 2015.
(Teaching Assistant)

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 différents 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

<http://www.debian.org>

2006 to present.

- 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

3H Avenue, Salto Angel Mall, Office 1. Maracaibo, Venezuela

May 2009 to June 2010.

- 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

Las Margaritas Street, La Asunción.
Margarita Island, Venezuela.

October 2008 to July 2009.

- 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.

LANGUAGES

Spanish, Mother language. —

English, Advanced English for Adults. 2006 to 2008.
Centro Venezolano Americano del Zulia (CEVAZ).
Maracaibo, Venezuela.

French, Elemental Course. 2010.
Alliance Française.
Maracaibo, Venezuela.

French, Advanced Course. 2013.
Alliance Française.
Toulouse, France.

PRESENTATIONS, PROCEEDINGS & SEMINARS

Scientific

- 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*. 21st to 27th July, 2018. West Dover, VT, United States.
- Oral presentation: “Acceleration of Saddle-Point Searches Assisted by Machine Learning”. The 68th Annual Meeting of the International Society of Electro-chemistry. 31st 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 50th *Symposium on Theoretical Chemistry 2014 (STC 2014)* held from 14th to 18th 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 1st to 4th 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 22nd 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 1st to 5th 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 6th to 7th June, 2013. Le Barcarès, France.
- Poster presentation: “The behavior of the Position-Spread Tensor in Diatomic Systems” in the 7th Molecular Quantum Mechanics (MQM) congress held from the 2nd to the 7th June, 2013. Lugano, Switzerland.
- Attendee to the “Theoretical Chemistry For Periodic Systems: Systematically Improvable Electronic Structure Methods (SIMPS 2013)” held from the 11th to the 15th 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 Respetivos 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. Altigracia. 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 Bellosó 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. 1st July, 2014. Badajoz, Spain.
- CECAM Theoretical Chemistry and Computational Modelling, Winter School on Large Systems (QCLAMS 2014). Saint-Lary-Soulan, France. January 20th-24th, 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”. 5th 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”. 26th June, 2012. University of Barcelona.
- 6th 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 machine learning library.
- Medium skills on the usage of scikit-learn machine learning package.
- FireWorks open-source code for defining, managing, and executing workflows.
- MongoDB databases.
- Skills on writing in the high-quality typesetting system, L^AT_EX.
- Programming languages: Python, FORTRAN 77, FORTRAN 90,
- BASH scripting.
- Skills on computational quantum mechanical programs such as: GPAW, MOLPRO, Gaussview, Gaussian, Molden, Chimera, Jmol, Materials Studio, Molekel, 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).

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 H₄⁺ 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

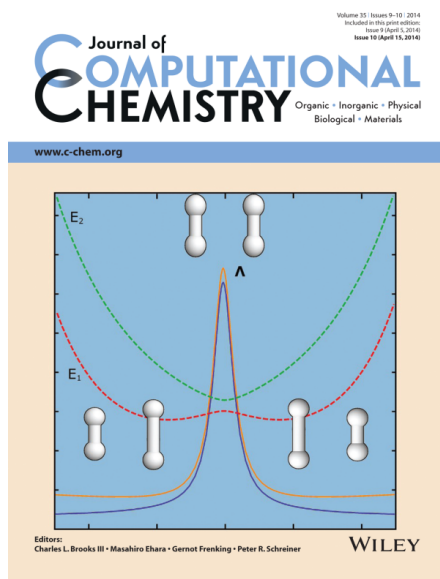


Figure 1: The $(\text{H}_2-\text{H}_2)^+$ system exhibits a mixed-valence character when the two hydrogen dimers are sufficiently apart, with the hole localized on the dimer with the longest bond. The cover shows energies of the two lowest electronic states (dashed lines) as a function of a reaction 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.

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.
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

INTERESTS

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