

JOSÉ G. PARRA

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University of Carabobo. FACYT. Chemistry Department. Physical chemistry Academic Unit.
Computational Chemistry Laboratory (QUIMICOMP). Av. Salvador Allende, Bárbula-Venezuela.



PROFESSIONAL PROFILE

Doctor of Sciences, mention in chemistry, in the area of physical chemistry obtained in the Postgraduate in Chemistry of the Sciences Faculty, Central University of Venezuela (UCV) in June 2017. At this time, I am developing investigation projects to study the interfacial properties of different mixtures of surfactants located in the interfacial regions of the vapor-liquid, liquid-liquid and liquid-solid systems using computational techniques such as molecular dynamics and mesoscopic dynamics. Also, in the use of ab-initio and DFT methods to study the chemical kinetics of organic reactions in vacuum and different solvent media. Similarly, in the use of the computational techniques QM-MM, FMO-MM and EFP-MM for the prediction of the solubility of organic compounds and pharmaceutical products in different organic solvents. Also, I am dedicated to the study of the local diffusion of molecules with pharmaceutical properties and natural products through lipid membranes.

<https://orcid.org/0000-0001-5991-3152>,

<https://www.scopus.com/authid/detail.uri?authorId=54412950400>,

<https://scholar.google.co.ve/citations?user=fs-FRv4AAAAJ&hl=es>

EDUCATION

Central University of Venezuela (UCV), Sciences Faculty, Postgraduate in Chemistry,
Physical Chemistry, Caracas-Venezuela *June, 2017*

Doctor of Sciences, mention in Chemistry

Advisory Researcher:

Dr. Yosslen R. Aray, IVIC Senior Researcher, IVIC-Venezuela.

Doctoral thesis entitled:

Study of water/surfactant/oil and solvent/surfactant/rock systems using molecular dynamics techniques

University of Carabobo,
Faculty of Education Sciences,
Direction of Postgraduate,
Postgraduate of the Faculty of Education Sciences.
Bárbula-Venezuela

Cohorte 2005-3

Extension Course and Teacher Training

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry, Bárbula, Venezuela.

December, 2002

Graduated in Chemistry

Advisory Researcher:

Dr. José Guaregua, University of Carabobo

Degree thesis entitled:

Correlation between the molecular structure of surfactants and their hydrophilic-lipophilic balance (HLB)

High School Alfredo Pietri, San Joaquín-Venezuela

October, 1997

Bachelor in Sciences

PROFESSIONAL EXPERIENCE

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Full Titular Professor

June 2022-December 2023

Bárbula-Venezuela

- Courses: Physical chemistry I, II y III; General chemistry I y II; Introduction to Molecular Simulation of Complex Systems.
- Research area: Computational Chemistry, Polymers, Surface Phenomena and Colloidal Chemistry.

NC state University,
Materials and Engineering, Department of Forest Biomaterials,
Department of Chemistry,
Computational Chemistry, Visiting Research/Remote, PAL Research Group NC State, Raleigh

March 2022-March 2023

- Research area: Computational Chemistry, Polymers, Cellulose and Colloidal Chemistry.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Professor of the Doctorate in Technological Chemistry

October 2017-December 2022

Bárbula-Venezuela

- Directed courses: Computational Methods of Molecular Simulation; Molecular Dynamics for the Prediction of Experimental Properties.
- Research area: Computational Chemistry, Polymers, Surface Phenomena and Colloidal Chemistry.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Research Associate Professor

June 2017-December 2020

Bárbula-Venezuela

- Courses: Physical chemistry I, II y III; General chemistry I y II; Introduction to Molecular Simulation of Complex Systems.

- Research area: Computational Chemistry, Polymers, Surface Phenomena and Colloidal Chemistry.

National Autonomous University of Mexico,
Materials Research Institute (IIM),
Visiting researcher

February, 2018-March, 2018
Mexico City, Mexico

- National Autonomous University of Mexico,
Materials Research Institute (IIM) under the supervision of Dr. Hector Dominguez,
Mexico City, Mexico.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Research Aggregate Professor

April, 2012-June, 2017
Bárbula-Venezuela

- Courses: Physical chemistry I, II y III; General chemistry I y II; Introduction to Molecular Simulation of Complex Systems.
- Research area: Computational Chemistry, Polymers, Surface Phenomena and Colloidal Chemistry.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Research Assistant Professor

October, 2007-June, 2012
Bárbula-Venezuela

- Courses: Physical chemistry I, II y III; General chemistry I y II; Introduction to Molecular Simulation of Complex Systems.
- Research area: Computational Chemistry, Polymers, Surface Phenomena and Colloidal Chemistry.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Instructor Professor

August, 2004-October, 2007
Bárbula-Venezuela

- Courses: Physical chemistry I, II y III; General chemistry I y II; Introduction to Molecular Simulation of Complex Systems.
- Research area: Computational Chemistry, Polymers, Surface Phenomena and Colloidal Chemistry.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Hired Instructor Professor

October, 2003-August, 2004
Bárbula-Venezuela

- Courses: Analytical Chemistry and General and Analytical Chemistry Laboratory.
- Research area: General and Analytical Chemistry.

University Institute of Industrial Administration Technology, IUTA
2004
Hired Instructor Professor.

April, 2002-May,
Bárbula-Venezuela

- Courses: Introduction to Industrial Hygiene and Safety, Geology, Petroleum Laboratory.

University of Carabobo,
Experimental Faculty of Sciences and Technology,

Department of Chemistry,
Physical Chemistry Laboratory Assistant.

August, 2001-December, 2002
Bárbula- Venezuela

- Course: Physicochemistry Laboratory.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Laboratory Assistant of General and Analytical Chemistry.

July, 2000-August, 2001
Bárbula- Venezuela

- Course: Laboratory of General and Analytical Chemistry.

ADMINISTRATIVE MANAGEMENT

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Coordinator of the Physical Chemistry Academic Unit of the Department of Chemistry
Bárbula- Venezuela

February, 2020-Actually.

- Evaluate, coordinate and plan the teaching and research activities of the teaching staff of the Chemistry Department in the physical chemistry academic unit.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Career Coordinator of the Chemistry Department

September, 2016-June-2018
Bárbula- Venezuela

- Supervise the teaching activities of the teaching staff of the Department of Chemistry.
- Evaluate the academic programs of the courses in the Department of Chemistry.
- Supervise the enrollment processes in the different semesters of the Chemistry degree.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Coordinator of Degree Thesis of the Department of Chemistry

February, 2016-September, 2016
Bárbula- Venezuela

- Coordinate and enforce the administrative procedures associated with the preparation and presentation of projects and thesis for the degree in chemistry.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Coordinator of the Physical Chemistry Academic Unit

October, 2012-December, 2014
Bárbula- Venezuela

- Evaluate, coordinate and plan the teaching and research activities of the teaching staff of the Chemistry Department in the physical chemistry academic unit.

RESEARCH PROJECTS

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Participant

April,2020-Abril,2021
Bárbula- Venezuela

- Title of the project: Surfactant molecules for gas adsorption by computer simulations.

- Developed at the University of Carabobo, Experimental Faculty of Sciences and Technology, Department of Chemistry, Barbula-Venezuela in collaboration with Dr. Hector Dominguez of the Materials Research Institute (IIM) of the National Autonomous University of Mexico, UNAM.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Coordinator

January,2020-Actually
Bárbula- Venezuela

- Title of the project: Evaluation of the physicochemical variables involved in the formulation of microemulsions through molecular dynamics simulations
- Developed at the University of Carabobo, Experimental Faculty of Science and Technology, Department of Chemistry, Barbula-Venezuela with the collaboration of Dr. Peter Iza of the Faculty of Natural Sciences of the Polytechnic School of the Litoral, Guayaquil, Ecuador

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Coordinator

October,2018-October,2019
Bárbula- Venezuela

- Title of the project: Study of the effect of nonionic surfactants on the stability of ionic surfactant foams through molecular dynamics simulations.
- Developed at the University of Carabobo, Experimental Faculty of Sciences and Technology, Department of Chemistry, Barbula-Venezuela with the collaboration of Dr. Peter Iza of the Faculty of Natural Sciences of the Polytechnic School of the Litoral, Guayaquil, Ecuador.

National Autonomous University of Mexico,
Materials Research Institute (IIM),
Mexico City-Mexico

February, 2018-Marzo, 2018

- Title of the project: Study of the effect of nonionic surfactants on the stability of ionic surfactant foams through molecular dynamics simulations.
- Developed at the National Autonomous University of Mexico, Institute for Materials Research (IIM) under the supervision of Dr. Hector Dominguez, Mexico City, Mexico.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Coordinator

March,2006-March, 2007
Bárbula- Venezuela

- Title of the project: Mesoscopic study of Polyethylene Oxide (PEO) solutions in water using diffusive particle dynamics (DPD).
- Developed at the University of Carabobo, Experimental Faculty of Sciences and Technology, Department of Chemistry, Barbula-Venezuela with the supervision of Dr. Yosslen Aray, IVIC Senior Researcher, Altos de Pipe, Edo. Miranda.

University of Carabobo,
Experimental Faculty of Sciences and Technology,
Department of Chemistry,
Participant

December,2005-December,2008
Bárbula- Venezuela

- Title of the project Nanometric and mesoscopic modeling of the interactions involved in the rock-oil-aqueous phase system as a tool to assist the recovery and transport of heavy crude oils. Project FONACYT-G-2005000424.
- Developed at the University of Carabobo, Experimental Faculty of Sciences and Technology, Department of Chemistry, Barbula-Venezuela, under the supervision of Dr. Yosslen Aray, IVIC Senior Researcher, Altos de Pipe, Edo. Miranda.

PUBLICATIONS

1. Gabriela L. Galarza-Acosta, José G. Parra, Raiza Hernández-Bravo, Peter Iza, Eduardo Schott, Ximena Zarate, Jimmy Castillo, Vladimiro Mujica, A Computational Chemistry Approach to the Molecular Design of SiO₂ Nanoparticles Coated with Stearic Acid and Sodium Stearate in Ethanol Solvent., *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, Volume 679, 2023, 132527.
<https://doi.org/10.1016/j.colsurfa.2023.132527>.
2. José G. Parra, Geraldine Rodriguez, Peter Iza, Ximena Zarate, Eduardo Schott (2023) Evaluation of the affinity of asphaltene molecular models A1 and A2 by the water/oil interfaces based on a novel concept of solubility parameter profiles obtained from MD simulations. *Journal of molecular liquids*, 376, 121430.
<https://doi.org/10.1016/j.molliq.2023.121430>.
3. Raiza Hernández-Bravo, Alma D. Miranda, José G. Parra, Juan M. Alvarado-Orozco, José M. Domínguez-Esquível, Vladimiro Mujica (2022) Experimental and Theoretical Study on the Effectiveness of Ionic Liquids as Corrosion Inhibitors. *Computational and Theoretical Chemistry*, 1210, 113640.
<https://doi.org/10.1016/j.comptc.2022.113640>.
4. José G. Parra, Peter Iza, Hector Dominguez, Eduardo Schott y Ximena Zarate. (2020) Effect of Triton X-100 surfactant on the interfacial activity of ionic surfactants SDS, CTAB and SDBS at the air/water interface: A study using molecular dynamic simulations. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 603, 125284.
<https://doi.org/10.1016/j.colsurfa.2020.125284>.
5. Yosslen Aray, José G. Parra, Ricardo Paredes, Luis Javier Alvarez, Antonio Diaz-Barrios. (2020) Exploring the nature of the interactions between the molecules of the sodium dodecyl sulfate and water in crystal phases and in the water/vacuum interface. *Heliyon*, 6, e04199, 1-12.
<https://doi.org/10.1016/j.heliyon.2020.e04199>.
6. José G. Parra, Hector Dominguez, Yosslen Aray, Peter Iza, Ximena Zarate y Eduardo Schott. (2019) Structural and interfacial properties of the CO₂-in-water foams prepared with sodium dodecyl sulfate (SDS): A molecular dynamics simulation study. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 578, 615.
<https://doi.org/10.1016/j.colsurfa.2019.123615>.
7. José G. Parra, Yosslen Aray, Peter Iza, Ximena Zarate y Eduardo Schott. (2019) Behavior of the SDS/1-butanol and SDS/2-butanol mixtures at the water/n-octane interface through Molecular Dynamics Simulations. *Chemical Physics*, 523, 138-149.
<http://dx.doi.org/10.1016/j.chemphys.2019.04.02>.
8. Miguel A. Díaz, José G. Parra, David S. Coll. (2017) Computational study of one-step polar Diels-Alder reactions using the NEB method for the minimum energy paths search. *Molecular Simulation*, 43(8), 644-655.
DOI: 10.1080/08927022.2017.1287910.

9. Yosslen Aray, José G. Parra, Doris Jimenez, Ricardo Paredes, Alejandro Martiz, Samantha Samaniego, Mauricio Cornejo, Eduardo Ludena, Cecilia Paredes. (2017). Exploring the Effect of the O-(1-heptylnonyl) Benzene Sulfonate Surfactant on the Nature of the Lineal Hydrocarbons/Water Interface by Means of an Atomistic Molecular Dynamic Simulation. *Journal of computational methods in sciences and engineering*, 17, 1, 39-53.
DOI: 10.3233/JCM-160659.
10. Yosslen Aray, Raiza Hernández-Bravo, José G. Parra, Jesús Rodríguez y David S. Coll. (2011). Exploring the structure-solubility relationship of asphaltene models in toluene, heptane, y amphiphiles using a molecular dynamic atomistic methodology. *Journal of Physical Chemistry A*, 115, 11495-11507.
<https://doi.org/10.1021/jp204319n>.

Disclosure Articles

1. Parra, José G.; González, José, Iza, P. y Perozo, E. (2023, enero-marzo). Un procedimiento para la obtención de los espectros IR, Raman y RMN de compuestos orgánicos mediante cálculos mecánico-cuánticos con el software ORCA-5.0.3. *Educación Química* 34(1):20-32.
<http://dx.doi.org/10.22201/fq.18708404e.2021.3.76027>
2. Miguel Á. Carrillo Hernández; Wilson H. Hirota y Parra, José G. Comportamiento de la amoxicilina en agua mediante métodos de solvatación implícita y explícita. *Rev. Colomb. Quim.*, vol. 51, no. 2, pp. 25-34, 2022.
<https://doi.org/10.15446/rev.colomb.quim.v51n2.103567>
3. Parra Figueredo, J. G., Iza, P. and Perozo, E. (2021, julio-septiembre). A guide to estimating the interfacial tension and interface thickness of a water/hydrocarbon system using the program gromacs-4.5.4. *Educación Química* 32(3):80-94.
<http://dx.doi.org/10.22201/fq.18708404e.2021.3.76027>
4. José G. Parra, Yosslen R. Aray, Peter Iza, Geraldine Rodriguez, Elizabeth Perozo. (2019) Distribution of 1-butanol and 2-butanol in water/n-octane and water/Sodium Dodecyl Sulfate (SDS)/n-octane systems using molecular dynamics. Part II. Using the gmx-density and gmx-densmap tools. *ACI Avances en Ciencias e Ingeniería*, 11(17), 172-189.
<http://dx.doi.org/10.18272/aci.v11i2.1289>.
5. José G. Parra, Yosslen R. Aray. (2016). Behavior of SDS located in the water/n-octane interfacial region. A study using molecular dynamics. *ACI Avances en Ciencias e Ingeniería*, 8(14), 98-110.
<http://dx.doi.org/10.18272/aci.v8i1.279>.
6. José G. Parra, Yosslen R. Aray, José A. Alcalá, Geraldine Rodriguez. (2014) Effect of sodium dodecyl sulfate (SDS) on interfacial film thickness and molecular orientation of water in water/1-pentanol and water/1-hexanol systems. *Faraute de Ciencias y Tecnología*, 9, 1, 5-11.
7. José G. Parra, Yosslen R. Aray. (2014). Molecular Dynamics Simulations of 1-butanol and 2-butanol located at the n-hexane/water, cyclohexane/water and toluene/water interfaces. *Avances en Química*, 9(3), 87-96.
<https://www.redalyc.org/articulo.oa?id=93333720001>.
8. José G. Parra, Yosslen R. Aray. (2011). Prediction of Molar Volume and Molar Enthalpy of Vaporization of organic molecules using variables determined by the

COSMO model. *Avances en Química*, 6(3), 79-88.
<http://www.saber.ula.ve/handle/123456789/34545>

9. José G. Parra, Yosslen R. Aray. (2011). Relationship between the cohesive energy density of hydrocarbons, linear alcohols and aromatic compounds with the non-bonding free energy density estimated by solvation methods. *Faraute de Ciencias y Tecnología*, 6(2), 12-21.
10. José G. Parra, José Guaregua, Yosslen R. Aray. (2010). Estimation of the Solubility Parameter of models of fractions A1 and A2 of asphaltenes through molecular dynamics. *Faraute de Ciencias y Tecnología*, 5(1), 68-76.

CONGRESSES AND SCIENTIFIC EVENTS

1. Barrios N., Parra J.G., Lucia L., Venditti R., Pal L. Unveiling the Cellulose-Water Interaction Through Computational Simulations (2023) TAPPICon 2023 - "Rock the Roll: Unleashing the Harmonies of the Paper Industry", Conference paper.
2. José G. Parra, Myleidys Paredes and Peter Iza. A theoretical study of the nitration of Imidazole in gas phase. The Royal Society of Chemistry 2022, RSCPoster Twitter Conference. Poster speaker, 2 y 3 de March, 2022.
3. José G. Parra, Peter Iza. DFT study of the reaction of 1,3-Cyclopentadiene with MVK in certain solvents. XIX Mexican Meeting of Theoretical Physicochemistry 2021, Poster speaker, CompChem. November, 2021.
4. Jose G. González A., José G. Parra, Peter Iza. Exploring the hydrogen bond type interactions in organic compounds with pharmaceutical properties using molecular simulation method. LatinXchem, Chemistry Twitter Poster Conference 2021, Poster speaker, CompChem. September, 2021.
10.26226/morressier.616e5c2462ba8657678b1311
5. José G. Parra, Peter Iza, Hector Dominguez, Mariangeles Salas. Molecular aggregation of Muricatacin in water using MD simulations. LatinXchem, Chemistry Twitter Poster Conference 2021, Poster speaker, CompChem. September, 2021.
DOI:10.26226/morressier.616e5c2462ba8657678b1329.
6. Mariángeles Salas, José G. Parra, Peter Iza. Molecular dynamics simulations of the molecular interaction of muricatacin with a charged phospholipid membrane. LatinXchem, Chemistry Twitter Poster Conference 2021, Poster speaker, PhysChem. September, 2021.
DOI:10.26226/morressier.616e5c2462ba8657678b1393.
7. José G. Parra, Hector Dominguez and Peter Iza. Effect of NaCl on the Adsorption of SDBS Surfactant at the Water/nOctane Interface With Presence of Linear Alcohols. A Study Using MD Simulations. The Royal Society of Chemistry 2021, RSCPoster Twitter Conference. Poster speaker, 2 y 3 de March, 2021.
8. Mariángeles Salas, José G. Parra, Peter Iza, Ximena Zarate, Eduardo Schott. Molecular Dynamics Simulations of the Molecular Interaction of Muricatacin with Phospholipids Membranes. The Royal Society of Chemistry 2021, RSCPoster Twitter Conference. Poster speaker, 2 y 3 de March, 2021.
9. José G. Parra and Peter Iza. Computational theoretical study of reaction path of the unimolecular decomposition of malonic acid in the gas phase using the NEB method. LatinXchem, Chemistry Twitter Poster Conference 2020. Poster speaker, TheoChem. September, 2020. DOI: 10.26226/morressier.5f6c5f439b74b699bf390c31.

10. José G. Parra, Peter Iza and Hector Dominguez. Molecular packing of SDS surfactant at the air/water interface by means of MD simulations. An estimation of the area per molecule occupied by the SDS surfactant. LatinXchem, Chemistry Twitter Poster Conference, 2020. Poster speaker, ChemPhys. September, 2020.
11. José González and José G. Parra. Computational prediction of C^{13} chemical shifts of benzoic acid. LatinXchem, Chemistry Twitter Poster Conference, 2020. Poster speaker, TheoChem. September, 2020.
12. José G. Parra. Molecular dynamics simulations to study synergism between SDS/1-butanol and SDS/2-butanol mixtures located at the interfacial region of water/n-octane system. 4th International Conference on Materials Science, ICMS 2017. Poster speaker. Valdivia-Chile. October, 2017.
13. José G. Parra. Affinity of asphaltene models of Venezuelan crude oils to water/oil interfaces. A molecular dynamics study. 4th International Conference on Materials Science, ICMS 2017. Ponente Cartel. Valdivia-Chile. October, 2017.
14. José G. Parra, Yosslen R. Aray. Determination of the lateral diffusion of asphaltene models in water/n-heptane and water/toluene by molecular dynamics. IV Venezuelan Congress of Science, Technology and Innovation within the framework of the LOCTI and PEII. Speaker Poster. Basic sciences. Caracas Venezuela. December, 2015.
15. Geraldine Rodríguez, José G. Parra. Behavior of certain asphaltene models in different organic solvents by computational techniques. IV Venezuelan Congress of Science, Technology and Innovation within the framework of the LOCTI and PEII. Speaker Poster. Basic sciences. Caracas Venezuela. December, 2015.
16. José G. Parra, Yosslen Aray. Molecular Dynamics Study of Sodium Dodecyl Sulfate (SDS) located in the water/1-pentanol and water/1-hexanol interfacial region. V Congress of Physicochemistry Theoretical and Computational, Venezuela-Edo. Miranda. December, 2014.
DOI:10.13140/RG.2.1.3689.2009.
17. José G. Parra, Geraldine Rodríguez, Dennis Cazar, Javier Torres. Molecular interactions between amino-g and water using continuous solvation and molecular dynamics methods. fifth congress of Theoretical and Computational Physicochemistry, Venezuela-Edo. Miranda. December, 2014.
18. José G. Parra, Yosslen Aray. Exploring the interfacial properties of the n-octane/SDS/water/SDS/n-octane system by molecular dynamics. III Venezuelan Congress of Science, Technology and Innovation within the framework of LOCTI and PEII. Speaker Poster. Basic sciences. Caracas Venezuela. November, 2014.
19. José G. Parra. Molecular dynamics simulation of C12E2 and C12 E5 surfactants located at the vacuum/water interface. II Venezuelan Congress of Science, Technology and Innovation within the framework of the LOCTI and PEII. Speaker Poster. Basic sciences. Caracas Venezuela. November 2013.
20. José G. Parra. VIII National Congress and 2nd. International Research Congress of the University of Carabobo. Coordinator of the session: Basic Sciences. Bárbula-Venezuela. November 2013.
21. José G. Parra, Yosslen Aray. Molecular dynamics simulation of sodium dodecyl sulfate surfactant located at the vacuum/water interface. VIII National Congress

- and 2nd. International Research Congress of the University of Carabobo. Speaker poster. Basic sciences. Valencia-Venezuela. November 2013.
22. José G. Parra, Yosslen Aray. IV Congress of Theoretical and Computational Physicochemistry. Simulation of the n-hexane/1-butanol/water system using molecular dynamics. Speaker Poster. Caracas Venezuela. November 2012.
 23. José G. Parra. Relationship between the solubility parameter and the non-bonding free energy density of some solvents estimated using the C-PCM solvation method. VII National Congress and 1st. International Research Congress of the University of Carabobo. Oral Speaker. Valencia-Venezuela. December, 2010.
 24. José G. Parra. IX Venezuelan Congress of Chemistry and I International Congress of the Venezuelan Chemistry Society. Coordinator of the session: Theoretical Chemistry I. Cumaná-Venezuela. June, 2009.
 25. José G. Parra, Angelesmary Roldán. Study of the solubility of models of fractions A1 and A2 of asphaltenes through molecular dynamics. IX Venezuelan Congress of Chemistry and I International Congress of the Venezuelan Society of Chemistry (SVQ). Oral Speaker. Cumaná-Venezuela. June, 2009.
 26. José G. Parra, Genny Galvis. Estimation of the interaction energies of asphaltene fractions models on dolomite (001) and magnesite (100) surfaces by molecular dynamics. VI Research Congress of the University of Carabobo. Oral Speaker. Valencia-Venezuela. October, 2008.
 27. José G. Parra, José Guaregua. Correlation between the molecular structure of surfactants and their lipophilic-hydrophilic character (HLB). VII Venezuelan Congress of Chemistry of the Venezuelan Chemistry Society. Oral Speaker. Mérida-Venezuela. November, 2005.
 28. José G. Parra. 1st Conference on initiation to research for FACYT students. University of Carabobo, Experimental Faculty of Sciences and Technology. Oral Speaker. Valencia-Venezuela. October, 2002.

DATA MENDELEY

1. José G. Parra, Peter Iza, Hector Dominguez, Eduardo Schott y Ximena Zarate (2020), Final configuration of surfactants in mixed monolayer in "Effect of Triton X-100 surfactant on the interfacial activity of ionic surfactants SDS, CTAB and SDBS at the air/water interface: A study using molecular dynamic simulations", Mendeley Data, VI,
<http://dx.doi.org/10.17632/m66dsvpnp7.1>
2. José G. Parra, Peter Iza, Hector Dominguez, Ximena Zarate, Eduardo, Schott (2020), Reparametrization of vdW parameters between Water and CO₂ force fields using solvation free energy in "Structural and interfacial properties of the CO₂-in-water foams prepared with Sodium Dodecyl Sulfate (SDS): A Molecular Dynamics Simulation study", Mendeley Data, VI,
<http://dx.doi.org/10.17632/78fvhhscy8.1>

ABILITIES AND SKILLS

a) Office Software

1. Linux and Windows operating systems
2. Microsoft office (MS Word, PowerPoint, MS Excel)

3. Libre office (Writer, Impress, Calc)
 4. Latex Editor (Texmaker y Texlive)
- b) Molecular Simulation software
1. Molecular dynamics software (GROMACS, Materials Studio, DL-POLY, LAMMPS)
 2. Quantum Chemistry software (GAMESS-US, GAUSSIAN, ORCA, Materials Studio)
 3. Molecular visualization software (Visual molecular Dynamics, Chimera, Multiwfn, Avogadro, Jmol y Gabedit)
- c) Instrumentation and Equipment
1. Gas chromatography and HPLC equipment.
 2. Infrared spectroscopy equipment.
 3. UV-Visible spectroscopy equipment.
 4. Potentiometry and Conductometry equipment.
 5. Equipment for automatic titration Metrohm brand.
 6. Du-Nouy and Wilhelmy tensiometer.

REVIEWER OF SCIENTIFIC ARTICLES AND EDITORIAL BOARD

1. Editorial board membership. International Journal of Computational and Theoretical Chemistry(IJCTC). ISSN Print: 2376-7286, <http://www.sciencepublishinggroup.com/j/ijctc>.
2. Avances en Ciencias e Ingeniería (ISSN:0718-8706). La Serena-Chile, trabajo ACI1223-14. Noviembre, 2014.
3. Journal of Computational Methods in Science an Engineering JCMSE (www.iospress.nl). Diciembre, 2015.
4. Journal of Molecular Structure. Elsevier, Amsterdam, The Netherlands. Junio, 2016.
5. International Journal of Biochemistry Research and Review. Science domain international. Enero, 2017.
6. Asian Journal of Physical Chemistry and Chemical Science. Science domain international. Abril, 2017.
7. Asian Journal of Physical Chemistry and Chemical Science. Science domain international. Octubre, 2018.
8. Asian Journal of Research and Reviews in Physics. Science domain international. Enero, 2019.
9. Chemical Science International Journal. Science domain international. Febrero, 2019.
10. Asian Journal of Applied Chemistry Research. Science domain international. Diciembre, 2019.
11. Revista Heliyon, Editorial Elsevier. Febrero, 2019.
12. Revista Energy and Fuels, American Chemical Society. Marzo, 2020.

13. Chemical Science International Journal. Science domain international. Enero, 2020.
14. Physical Science International Journal. Science domain international. Febrero, 2020.
15. Colloids and Surfaces A: Physicochemical and Engineering Aspects, Editorial Elsevier. Junio, 2020.
16. Chemical Engineering Science, Editorial Elsevier. Julio, 2020.

DICTATED CONFERENCES

1. Chemical education towards a technical approach. 1st Chemistry Symposium. University of Carabobo, Faculty of Education, Department of Biology and Chemistry. Bárbula-Venezuela. January, 2015.
2. Continuous solvation and molecular dynamics methods applied to predict the solubility of organic compounds. V Congress of theoretical and computational physicochemistry. IVIC, Altos de Pipe- Venezuela. December, 2014.
3. Molecular dynamics and continuous solvation methods applied to complex systems. Higher Polytechnic School of the Coast (ESPOL), Faculty of Natural Sciences, Guayaquil-Ecuador. October, 2014.
4. Evaluation of the interfacial properties between sodium dodecyl sulfate and the alcohols 1-butanol and 2-butanol located at the water/n-octane interface by molecular dynamics. Materials Research Institute, National Autonomous University of Mexico, Mexico City, February, 2018.

DICTATED COURSES

1. Fundamentals and applications of Molecular Dynamics and Training and use of the GRONigen MACHines Simulations Program (GROMACS). Department of Physics of the Faculty of Natural Sciences and Mathematics of ESPOL Guayaquil-Ecuador. October, 2014.
2. Simulation of complex systems using molecular dynamics. Guest instructor at the 2nd. School of Theoretical and Computational Chemistry of the Americas-PREFALC 2014. San Francisco de Quito University-Ecuador. July, 2014.

UNDERGRADUATE THESIS DIRECTION

1. Study of the behavior of A1 and A2 fractions of asphaltenes in different organic solvents using molecular dynamics. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2007.
2. Evaluation of adsorption energies of asphaltene fractions on carbonate rock surfaces by molecular dynamics. University of Carabobo. Faculty of Engineering. School of Chemistry. Year: 2008.
3. Evaluation of the solubility of asphaltenes through mesoscopic dynamics. University of Carabobo. Faculty of Engineering. School of Chemistry. Year: 2008.
4. Modelling the adsorption of resins with various functional groups on alumina and hematite using molecular dynamics. University of Carabobo. Faculty of Engineering. School of Chemistry. Year: 2008.
5. Study of the effect of dielectric constant on the estimation of density and the solubility parameter of pure organic solvents, models of asphaltenes and neutral surfactants. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2009.

6. Adsorption of organic molecules on the surface of beta-quartz using methods of molecular mechanics and dynamics. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2010.
7. Ab-initio study of the hydrogen bonds type intermolecular interaction of linear alcohols. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2012.
8. Adsorption of asphaltene fractions models in organic solvents (n-heptane and toluene) on calcite surface by molecular mechanics and dynamics techniques. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2012.
9. Estimation of the distribution of nonionic surfactants in biphasic systems using solvation methods. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2012.
10. Correlation between the experimental solubility of naphthalene in different organic solvents and the interaction energy calculated with ab-initio methods. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2012.
11. Estudio de la formación de monocapas y agregación en agua de los surfactantes catiónicos bromuro y cloruro de n-alquil trimetil amonio. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2014.
12. Estimation of the interactions and properties of 1-butanol and 2-butanol with sodium dodecyl sulfate located at the n-octane/water interface by molecular dynamics. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2014.
13. Implementation of the NEB method in the theoretical study of Diels-Alder reactions in solution. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2016.
14. Exploring the behavior of the ionic surfactant sodium dodecyl sulfate (SDS) and its interactions in the water/1-pentanol and water/1-hexanol interfacial region using molecular dynamics. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2016.
15. Aggregation of the fractions of asphaltenes located in the water/toluene and water/n-heptane interfacial regions by molecular dynamics. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2016.
16. Study of the effect of the triton series on the interfacial properties of sodium dodecyl sulfate/water through molecular dynamics. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2016.
17. Solubility and preferential solvation of sulfamerazine and sulfamethazine using molecular dynamics. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2018.
18. Application of the QM/MM method on the reaction of 1,3-Cyclopentadiene with Methyl-vinyl-ketone in different solvents. A study of the Diels-Alder reaction in solution. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2018.

19. Computational study of the acid-base behavior and molecular interactions of the structural model of humic acid TNB in aqueous solution. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2019.
20. Theoretical estimation of spectroscopic signals of pharmaceutical compounds. A computational study using the Density Functional Theory. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2021.
21. Evaluation of the molecular interaction between muricatacin and different phospholipid membranes using molecular dynamics. University of Carabobo, Experimental Faculty of Sciences and Technology. Department of Chemistry. Year: 2021.

COMPLETED COURSES

1. Aspects of toxic waste management. VI National Meeting of Science Students. Faculty of Sciences, UCV. October, 2001.
2. V Workshop of Methodological Advisors. University Institute of Technology for Industrial Administration, Valencia Extension. Duration: 8 hours. November, 2003.
3. Formation of effective Work Teams. Ministry for the Popular Economy, National Institute for Educational Cooperation. Duration: 8 hours. January, 2004.
4. Extension Course and Teacher Training. University of Carabobo, Faculty of Educational Sciences, Postgraduate Department. Duration: 288 hours. Cohort 2005-03.
5. Industrial Catalyst and Processes. Central University of Venezuela, Faculty of Sciences, Postgraduate in Chemistry. Duration: 30 hours. May, 2011.
6. How to peer review a review article. Researcher Academy, Elsevier. August, 2020.
7. Novel Approaches in GPCR Drug Design. Pharmacelera. 22 de Junio, 2021.

AWARDS AND HONOURS

1. Certificate of Recognition. Thank you for your valued contributions to ACS Publications. ACS Publications awards, 2020.
2. Researcher type A-2. Program to stimulate innovation and research (PEII). Ministry of Science, Technology and Innovation, Caracas-Venezuela. March, 2015.
3. Researcher type A-1. Program to stimulate innovation and research (PEII). Ministry of Science, Technology and Innovation, Caracas-Venezuela. March 2013.
4. Researcher Level I. Science and Technology Observatory of the University of Carabobo. CDCH. Naguanagua, 2016.
5. III Meeting of Science and Technology in the advice of the activity: Experiences in Chemical Processes. Recognition granted by the University Institute of Technology and Administration. Valencia, 2004.
6. 1st. Place at the 1st FACYT Student Research Initiation Conference. University of Carabobo, Experimental Faculty of Sciences and Technology. November, 2002.
7. 1st. Place. Best Average of the Bachelor's Degree in Chemistry (17.5 on a scale of 1 to 20). University of Carabobo, Experimental Faculty of Sciences and Technology. October, 1997.