



Orlando Villegas

Doctor in Physical-Chemistry

- ▶ i-CLeSH
- ▶ Venezuelan, male
- ▶ 17/03/1993, Caracas

Skills

Data Processing with Python 4+ yrs.

Molecular Dynamics simulations 4+ yrs.

Quantum chemistry calculations 3+ yrs.

Linux and Server

French B2

English A2

Machine Learning

Summary

I am Venezuelan, PhD in Physico-Chemistry from UPPA. I am currently doing a Post-Doc at the Institute of Chemistry for Life and Health Sciences (i-CLeHS) Paris, working on the modeling of photonastic materials. I am involved in molecular simulation and theoretical chemistry. Furthermore, I am a python developer, which has helped me in data analysis and processing throughout my career. As key points that define me, I love learning, I like challenges and overcoming them.

Work

04/2022 - to present

Researcher

Institute of Chemistry for Life and Health Sciences (i-CLeHS) UMR8060 CNRS.

Photonastic materials ▪ *Photo-switching process* ▪ *Molecular Dynamic* ▪ *DT-DFT*

“Modeling photonastic materials: insights from the molecular scale”

Education

11/2018 - 03/2022

PhD in Physical-Chemistry

Université de Pau et des Pays de l'Adour and Universidad Central de Venezuela. Co-supervised thesis, supervisors: Dr. **Isabelle Baraille**, and Dr **Sócrates Acevedo**.

Asphaltens ▪ *Nanoparticles* ▪ *Molecular Dynamic* ▪ *PMF*

Doctoral's thesis: “Study of the Molecular Dynamics of Interaction A1 and A2 Asphaltene Subfractions With Nanoparticles in Presence of Solvents”

Work that falls within the framework of the joint laboratory UCV, IPREM UPPA - IC2MC - CNRS - TotalEnergies.

11/2010 - 10/2018

Degree in Chemistry

Universidad Central de Venezuela. Supervisors: Dr. **Jimmy Castillo** and Dr. **Sócrates Acevedo**.







Asphaltens ▪ *Solubility* ▪ *Molecular Dynamic*

Thesis: “Study of the Solubility and Aggregation of Asphaltene Subfractions A1 and A2 using Molecular Dynamics Methods”

Publications

- Villegas, O., and Castillo, J. (2018). "Study of thermo-optical properties of nanofluids of gold and silver nanoparticles functionalized with polyethylene glycol and sodium dodecyl sulfate in water using thermal lens spectroscopy". *Proc. SPIE 10672, Nanophotonics VII*, 106723S, 256–261. <https://doi.org/10.1117/12.2307284>

Contact

-  11 rue Pierre et Marie Curie
75005 Paris - France
-  +33 7 80 54 24 15
-  orlando.villegas@chimieparistech
.psl.eu
-  0000-0003-2153-5840
-  github.com/ovillegasb
-  linkedin.com/in/ovillegasb

- Villegas, O., Salvato Vallverdu, G., Bouyssiére, B., Acevedo, S., Castillo, J., and Baraille, I. (2020). "Molecular Cartography of A1 and A2 Asphaltene Subfractions from Classical Molecular Dynamics Simulations". *Energy & Fuels*, 34(11), 13954–13965. <https://doi.org/10.1021/acs.energyfuels.0c02744>
- González, G., Acevedo, S. S., Castillo, J., Villegas, O., Ranaudo, M. A., Guzmán, K., Orea, M., and Bouyssiére, B. (2020). "Study of very high molecular weight cluster presence in THF solution of asphaltenes and subfractions A1, A2, by gel permeation chromatography with inductively coupled plasma mass spectrometry". *Energy & Fuels*, 34(10), 12535–12544. <https://doi.org/10.1021/acs.energyfuels.0c02743>

Congresses and conferences

- XIII Interamerican Microscopy Congress. **2015**. *MICROSCOPIC AND OPTIC CHARACTERIZATION OF Fe NANOPARTICLES PRODUCED BY NOVEL ELECTROCHEMICAL METHOD*. **Poster**.
- Photonic Europe, Strasbourg, France. **2018**. *STUDY OF THERMO-OPTICAL PROPERTIES OF NANOFUIDS OF GOLD AND SILVER NANOPARTICLES FUNCIONALIZED WITH POLYETHYLENE GLYCOL AND SODIUM DODECYL SULFATE IN WATER USING THERMAL LENS SPECTROSCOPY*. **Poster**.
- LXVIII Convención anual de la ASOVAC (Asociación Venezolana para el avance de la ciencias) november **2018**. *ESTUDIO DE LA SOLUBILIDAD Y AGREGACIÓN DE LAS FRACCIONES A1 Y A2 DE ASFALTENOS USANDO MÉTODOS DE DINÁMICA MOLECULAR*. **Oral Presentation**.
- Journée scientifique utilisateurs cluster Pyrene **2019**. *Molecular cartography of A1 and A2 asphaltens sub-fractions from classical molecular dynamics*. **Oral Presentation**.
- LXIX Convención anual de la ASOVAC (Asociación Venezolana para el avance de la ciencias) november **2019**. *AGREGACIÓN DE LAS SUBFRACCIONES DE ASFALTENO A1 Y A2 EN TOLUENO EMPLEANDO DINÁMICA MOLECULAR*. **Oral Presentation**.
- Conference **2020** LATINXChem. *Molecular Cartography of A1 and A2 Asphaltenes sub-fractions from classical molecular dynamic simulations*. **Poster**.
- PetroPhase **2021**. *Aggregation study of subfractions A1 and A2 of asphaltenes in different solvents*. **Poster**.
- ACS Fall **2021**. *Molecular cartography of asphaltens from classical molecular dynamics simulations*. **Oral Presentation**.