Associate Professor of Chemistry
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Luiz Oliveira

Professional experience

2020 - present **Associate Professor**, Department of Chemistry. Mount Vernon Nazarene University (MVNU), Mount Vernon - OH.

Research Computational Biophysics, Computational Materials Science

2018 - 2020 **Assistant Professor - Visiting**, Department of Chemistry. University of Cincinnati (UC), Cincinnati - OH.

Research Computational Biophysics

2015 - 2018 **Research Associate**, Department of Chemical Engineering. University of Washington (UW), Seattle - USA.

Research Molecular Modeling, Reaction Engineering

2013 - 2015 **Postdoctoral research fellow**, Laboratoire de Chimie et Physique Quantiques (LCPQ) and Laboratoire de Collision Agrégats et Réactivité (LCAR), Toulouse - France.

Research Computational Chemistry, Molecular Modeling

Education

2012 **Ph.D. in Chemistry**, University of Lyon and Atomic Energy and Alternative Energies Commission at Grenoble, France.

Title *Physical multiscale modeling of PEM water electrolyzers: from ab initio data to macroscale observables.*

Supervisors Professor Alejandro A. Franco & Professor Christian Jallut.

2008 **Master Degree in Physics and Materials Science**, *Double diploma* Ecole Normale Supérieure de Lyon - France *and* University of Roma "La Sapienza" - Italy .

2007 **B.S. Physics**, Universidade Federal de Uberlândia, Brazil.

Teaching

Individual Instruction

Current Undergraduate Researchers:

- Hannah Crouse (former XSEDE EMPOWER trainee) [2021 - present]
- Daniel Daly [2022 - present]
- Jerhett Morehouse [2023 - present]

Former Undergraduate Researchers:

- Alyssa Van Fossen (MVNU, XSEDE EMPOWER trainee) [Fall 2021]
- Ryan O'Donnel (MVNU, XSEDE EMPOWER trainee) [Summer and Fall 2021]
- Daniel Corcoran (UC) [2020 - 2021]
- Anupama Narayana (UC) [Fall 2019]
- Tien Do (UC) [Fall 2019]
- Tan Do (UC) [Fall 2019]
- Miwakoto Ito (UW) [Summer 2016]

Classroom Instruction

Mount Vernon Nazarene University:

Fall 2023

- CHE-2001: Special Topics: Computational Chemistry.
- CHE-4064: Physical Chemistry II with laboratory.
- CHE-1044: General Chemistry I with laboratory.
- MAT-4089: Special Topics: Data Science

Spring 2023

- CHE-1044: General Chemistry II with laboratory.
- CHE-4054: Physical Chemistry I with laboratory.

Fall 2022

- CHE-1034: General Chemistry I with laboratory.
- MAT-2063: Introduction to Statistics.

Spring 2022

- CHE-1044: General Chemistry II with laboratory.
- CHE-1060: General, Organic and Biochemistry laboratory.

Fall 2021

- CHE-1034: General Chemistry I with laboratory.
- CHE-2001: Special Topics: Introduction to Data Science.
- PHY-3010: Modern Physics Laboratory.

Spring 2021

- CHE-1044: General Chemistry II with laboratory.

Fall 2020

- CHE-1034: General Chemistry I with laboratory.

University of Cincinnati:

Summer 2020

- CHEM-1041: General Chemistry II. Online.

Fall 2019

- CHEM-1040: General Chemistry I.

Summer 2019

- CHEM-1040: General Chemistry I.

Fall 2018

- CHEM-1040L: General Chemistry I Laboratory.
- CHEM-1020L: Introduction to General, Organic and Biochemistry Laboratory.
- CHEM-1030L: Introduction to General, and Organic Chemistry Laboratory.

University of Washington:

Fall 2017

- ChemE-599. Molecular Modeling. Guest lecture: "Density functional theory methods and applications".

Spring 2016

- ChemE-599. Molecular Modeling. Guest lecture: "Parallel tempering molecular dynamics and metadynamics techniques".

Awards

- University of Washington - Office of Postdoctoral Affairs Travel Award. 2018
- Erasmus Mundus - AtoSim Master of Science Fellowship. 2007

Publications

- Hannah Crouse, Alyssa Van Fossen L. F. L. Oliveira, "Using metadynamics to determine the free energy landscaping of knotted proteins unfolding." *in preparation for PeerJ Physical Chemistry.*
- Daniel Daly, Binyang Hou, L. F. L. Oliveira, "Water Adsorption on Yttria-Stabilized Zirconia Surfaces" *in preparation for Surface Chemistry.*
- L. F. L. Oliveira, "Strategies for Effective Utilization of Writing and Educational YouTube Videos in the Context of General Chemistry Topics" *in preparation for the Journal of Chemical Education.*

- M Jora, D. Corcoran, G. Parungao, P. Lobue, L. F. L. Oliveira, G. Stan, B. Addepalli, P. Limbach "Higher-Energy Collision Dissociation Mass Spectral Networks for the Rapid, Semi-automated Characterization of Known and Unknown Ribonucleoside" *Analytical Chemistry*. (2022), 94, 40, 13958.
- H. Y. Fonseka, A. Javidi, L. F. L. Oliveira, C. Micheletti, and G. Stan. "Unfolding and translocation of knotted proteins by Clp biological nanomachines: synergistic contribution of primary sequence and topology revealed by molecular dynamics simulations" *J. Phys. Chem.* B (2021), 125, 27, 7335.
- K. S. Sykes, L. F. L. Oliveira, G. Stan, and R. J. White "Electrochemical Studies of Cation Condensation-Induced Collapse of Surface-Bound DNA" *Langmuir* (2019), 35, 40, 12962.
- L. F. L. Oliveira, C. D. Fu, and J. Pfaendtner. "Density Functional Tight-Binding and Infrequent Metadynamics can Capture Entropic Effects in Intramolecular Hydrogen Transfer Reactions" *J. Chem. Phys.* (2018) 148, 154101.
- C. D. Fu, L. F. L. Oliveira, and J. Pfaendtner. "Assessing Generic Collective Variables for Determining Reaction Rates in Metadynamics Simulations" *J. Chem. Theory Comput.* (2017), 13 (3), 968.
- C. D. Fu, L. F. L. Oliveira, and J. Pfaendtner. "Determining Energy Barriers and Selectivities of a Multi-Pathway System With Infrequent Metadynamics" *J. Chem. Physics* (2017), 146 014108.
- L. F. L. Oliveira, N. Tarrat, J. Cuny, J. Morillo, D. Lemoine, F. Spiegelman, and M. Rapacioli. "Benchmarking Density Functional Based Tight-Binding for Silver and Gold Materials: From Small Clusters to Bulk." *J. Phys. Chem. A*, (2016), 120 (42), 8469.
- L. F. L. Oliveira, J. Cuny, M. Moriniere, L. Dontot, A. Simon, F. Spiegelman, and M. Rapacioli. "Phase Changes of the Water Hexamer and Octamer in the Gas Phase and Adsorbed on Polycyclic Aromatic Hydrocarbons." *Phys. Chem. Chem. Phys.*, (2015), 17, 17079.
- L. F. L. Oliveira, C. Jallut, and A. A. Franco. "A Multiscale Physical Model of a Polymer Electrolyte Membrane Water Electrolyzer." *Electrochimica Acta*, (2013), 110, 363.
- L. F. L. Oliveira, E. Mayousse, C. Jallut, and A. A. Franco. "A Multiscale Physical Model for the Transient Analysis of PEM Water Electrolyzer Anodes." *Phys. Chem. Chem. Phys.*, (2012), 14, 10215.

Selected Presentations

Invited Talk

- "Water Adsorption on Transition Metal Oxide Pure IrO_2, RuO_2 and Alloy $Ru_xIr_{1-x}O_2$ Surfaces Investigated By Density Functional Theory."
  L. F. L. Oliveira, A. A. Franco, D. Loffreda.
  233rd Electrochemical Society Meeting. Seattle – US. May 2018.

Posters Presentations

- "Computational study of water tiltration through graphyne's pores."
  Hannah Crouse, L. F. L. Oliveira,
  Mercury conference – Greenville. July 2023.
- "Assessing the accuracy of density functional based tight-binding calculations for the structure and energetics of amino acids on gold nanoparticles."
  Jerheet Morehouse, L. F. L. Oliveira,
  Mercury conference – Greenville. July 2023
- "Calculating chemical reaction rates through metadynamics simulations."
  L. F. L. Oliveira, C. Fu, J. Pfaendtner
  Theory and Applications of Computational Chemistry – Seattle. August 2016.
- "Density functional theory study of the adsorption of water on the IrO_2(110), RuO_2(110) and $Ru_xIr_{1-x}O_2$(110) surfaces."
  L. F. L. Oliveira, C. Jallut, A. A. Franco and D. Loffreda.
  5^{th} International meeting of atomic and molecular physcis and chemistry (IMAMPC). Salamanca – Spain. June 2014.
- "Energetic and thermodynamical properties of pure water clusters on PAHs and of protonated water clusters."
  L. F. L. Oliveira, J. Cuny, M. Moriniere, L. Dontot, A. Simon, F. Spiegelman and M. Rapacioli.
  Meeting of the French Network of Theoretical Chemistry (RCTF). Paris – France. June 2014.
- "A multiscale physical model for the analysis of PEMWE from atomistic calculation up to macroscopic observables."
  L. F. L. Oliveira, C. Jallut, A. A. Franco.
  CECAM Workshop: Photo-meets Electrocatalysis: United We Split (...Water). Delmenhorst – Germany. October 2011.

Oral Presentations

- "Quantitative Calculation of Reaction Rates of Two Classes of Chemical Reactions by Infrequent Metadynamics Simulations."
  L. F. L. Oliveira, C. Fu, J. Pfaendtner.
  Materials Research Society Fall Meeting. Boston – US. November 2017.
- "DFT based tight binding strategy for numerous atoms studies: properties of noble metal clusters and surfaces interacting with hydrogen atoms."
  L. F. L. Oliveira, F. Spiegelman, M. Rapacioli and D. Lemoine.
  Thems GDR Meeting. Bordeaux – France. December 2014.
- "Energetic and thermodynamical properties of protonated water clusters and of water clusters adsorbed on polycyclic aromatic hydrocarbons."
  L. F. L. Oliveira, J. Cuny, M. Moriniere, L. Dontot, A. Simon, F. Spiegelman and M. Rapacioli.
  5^{th} International meeting of atomic and molecular physics and chemistry (IMAMPC). Salamanca – Spain. June 2014.

- "Investigation of atomic and molecular clusters with the DFTB approach."
  L. F. L. Oliveira, J. Cuny, M. Moriniere, L. Dontot, A. Simon, F. Spiegelman and M. Rapacioli.
  14^{th} deMon workshop. Los Cabos – Mexico. April 2014.
- "Multiscale modeling study of the electrochemical and transport mechanisms in PEM water electrolyzers."
  L. F. L. Oliveira, C. Jallut and A. A. Franco.
  63^{rd} Annual meeting of the international society of electrochemistry. Prague – Czech Republic. August 2012.

Service

- Member. Diversity Committee. MVNU
- Member. General Education Committee. MVNU
- Search Committee Member. HR Director. MVNU
- Faculty Search Committee Member. Music Faculty. MVNU
- Academic advisor. MVNU.
- Journal Referee, The Journal of Physical Chemistry.
- Group Manager, Pfaendtner Research Group, UW.
- Advisory Board, UW International Grad Student

Professional Development

- Member, American Chemical Society.
- Member, Molecular Education and Research Consortium in Undergraduate computational ChemistRY (MERCURY).
- Member, Midwest Undergraduate Computational Chemistry Consortium (MU3C).

Languages

Portuguese **Native**
English **Fluent**
French **Fluent**
Spanish **Conversational**