Laura Joana Silva Lopes

Name in bibliographic references LOPES, L. J. S. or LOPES, LAURA J. S.
E–mail laurajoanalopes@gmail.com **Skype** laurajoanalopes

Post–doctoral Fellow at Los Alamos National Laboratory

Skills

Computational Chemistry Development of sampling methods in MD, Molecular Dynamics (NAMD and LAMMPS), Force Field development, *ab initio* Methods (DFT)

Programming

Compiled C, C++, Fortran, CUDA, Pascal

Interpreted Bash, Tcl/Tk, Python, FreeFem++, Scilab, Matlab, Perl

Other LateX

Inorganic Chemistry Coordination compounds, Ultraviolet–visible Spectroscopy, X–ray Photoelectron Spectroscopy (XPS), X–ray Absorption Near Edge Structure (XANES), X–ray Diffraction, Catalysis

Languages

Portuguese native language

French fluent

English fluent

Education

2016–2019 PhD in Applied Mathematics CERMICS (ENPC) – Paris–Est University

Project *Numerical methods for the simulation of rare events in molecular dynamics*

Supervisors Tony Lelièvre and Jérôme Hénin

2015–2016 MSc (2nd year) Analysis, Modeling and Simulation Paris–Saclay University

2014–2015 MSc (1st year) Mathematics and mathematical engineering University of Versailles St–Quentin–en–Yvelines (UVSQ)

2011–2013 MSc Chemistry Federal University of Rio de Janeiro (UFRJ)

Project *SpeciFFic: Development and Application of a Program for Construction of Specific Force Fields*

Supervisor Marco Antonio Chaer Nascimento

Scholarship National Council for Scientific and Technological Development (CNPq)

2009–2010 BSc Physics Federal University of Rio de Janeiro (UFRJ)

2006–2008 BSc Chemistry (interrupted) Federal University of Rio de Janeiro (UFRJ)

Professional experience

Research

2021–now Los Alamos National Laboratory – Post–doctoral fellow

Project *Aiding the development of new potentials for fusion materials*

Supervisors Danny Perez and Nicholas Lubbers

2020–2021 University of Utah – Post–doctoral fellow

Project *Elucidating the Formation Mechanisms of Zeolites Using Data–Driven Modeling and In–Situ Characterization*

Supervisor Valeria Molinero

2016 **CERMICS (ENPC) – Internship for 2nd year Master's degree**

Project *Adaptive Multilevel Splitting Method: theoretical aspects and applications*

Supervisor Tony Lelièvre

2013–2014 **National Laboratory of Scientific Computation (LNCC) – Brazil**

Project *Construction of a Pipeline for identification of Repetitive Sequences in oysters of economic interest*

Supervisor Ana Tereza Ribeiro de Vasconcelos

Scholarship Reinforcement Program of Institutional Capacities from the Ministry of Science, Technology and Innovation (PCI–DC, Master level)

2008 **National Laboratory of Synchrotron Light (LNLS) – Brazil**

Project *XRD in situ in industrial catalysts: deployment of instrumentation and measurements of a HTS* catalyst

Supervisor Daniela Zanchet

Scholarship XVII Summer Scholarship Program

2006–2009 **Federal University of Rio de Janeiro (UFRJ)**

Project *Coordination Compounds of Copper and Cobalt with dithiolates*

Supervisors Nádia Maria Comerlato and Cássia Curan Turci

Scholarship Scholarship Program for Scientific Initiation from the National Council for Scientific and Technological Development (CNPq/PIBIC)

Teaching

2018 **Teaching Assistant** Mathematical tools for physics and electronics – (ESIEE – Paris)

2018 **Teaching Assistant** Differential Equations (programming course) – Pierre and Marie Curie University (UPMC)

2013–2014 **Lecturer** Chemistry I (laboratory course) – Distance Higher Education Centre of Rio de Janeiro State (CEDERJ)

2013 **Lecturer** Physics – Preparatory course for entrance exams to universities (PVS – CEDERJ)

2011 **Lecturer** Mathematics – Preparatory course for entrance exams to universities (PVS – CEDERJ)

2010 **Tutor** Computational Methods in Physics I – Federal University of Rio de Janeiro (UFRJ)

2010 **Tutor** Physics III – Federal University of Rio de Janeiro (UFRJ)

2009 **Tutor** Experimental Physics I – Federal University of Rio de Janeiro (UFRJ)

Scientific Production

Peer reviewed

1. HÉNIN, J., **LOPES, L. J. S.**, GIACOMO, F. *Human learning for molecular simulations: the Collective Variables Dashboard in VMD* Journal of Chemical Theory and Computation 18 (3), **2022**
2. BERTOLAZZO, A. A., DHABAL, D., **LOPES, L. J. S.**, WALKER, S. K., MOLINERO, V. *Unstable and Metastable Mesophases Can Assist in the Nucleation of Porous Crystals* The Journal of Physical Chemistry C 126 (7), **2022**
3. **LOPES, L. J. S.**, LELIÈVRE, T. *Analysis of the Adaptive Multilevel Splitting method on the isomerization of alanine dipeptide* Journal of Computational Chemistry 40 (11), **2019**
4. **LOPES, L. J. S.**, COMERLATO, N. M., GUERRA, A. C. O., TURCI, C. C., FERREIRA, G. B. *Vibrational and Electronic Spectroscopy of Neutral Antimony Coordination Compounds of the 1,3–Dithiole–2–thione–4,5–dithiolate (dmit)* The Journal of Physical Chemistry. A. 116 (9), **2012**
5. ZANCHET, D., RODELLA, C. B., **LOPES, L. J. S.**, LOGLI, M. A., VICENTINI, V. P., WEN, W., HANSON, J. C., RODRIGUEZ, J. A. *In situ time–resolved X–ray diffraction studies of Fe2O3 and Cu, Cr–Fe2O3 catalysts for the water–gas shift reaction* AIP Conference Proceedings 1092 (25), **2009**

Not peer reviewed

1. **LOPES, L. J. S.**, MAYNE, C. G., CHIPOT, C., LELIÈVRE, T. *Adaptive multilevel splitting method: Isomerization of the alanine dipeptide*, preprint, **2017**

Academic Distinctions

2022 Honorable Mention from Los Alamos National Laboratory
Work presented at the 2022 Science in 3 event
How to simulate materials in atomic scale for fusion energy reactors

2015 Scholarship from Fondation Mathématique Jacques Hadamard (Sophie Germain)
Scholarship earned by merit for the second year master's degree

2009 Honorable Mention from the Federal University of Rio de Janeiro
Presented work LOPES, L. J. S., FERREIRA, G. B., TURCI, C. C., COMERLATO, N. M. *Synthesis and spectroscopic characterization of Ni(II) complexes with dmit, dmio and dmt ligands* Event Giulio Massarani Convention for Scientific, Artistic and Cultural Initiation from UFRJ

Extracurricular activities

2017–2019 PhD students' representative at the CERMICS laboratory

2016–2018 Organizer of the PhD students' seminars at the CERMICS laboratory

2007–2009 Organizer of the Student's Chemistry Week at the Federal University of Rio de Janeiro (editions XV, XVI and XVII)

Invited Talks

1. **Laura Lopes**, Nicholas Lubbers, Danny Perez, *Using error models to take away redundancies from the training set: towards more transferable atomic potentials*, presented at SIAM Annual Meeting – Pittsburgh (PA–USA), July 11–15, 2022

2. **Laura Lopes**, Nicholas Lubbers, Danny Perez, *Estimation of errors in the prediction of long time scale properties with machine learning potentials for fusion materials*, presented at MRS Fall Meeting – Boston (MA–USA), November 29 to December 2, 2021

3. **Laura Lopes**, Jérôme Hénin, Tony Lelièvre, *A more efficient way to sample rare events through a combination of importance sampling and Adaptive Multilevel Splitting*, presented at the Minisymposium Metastable stochastic dynamics in materials: trajectory sampling and coarse–graining at the SIAM – MS21 (held online), May 17–28, 2021

4. **Laura Lopes**, Jérôme Hénin, Tony Lelièvre, *Simulation of rare events in molecular dynamics with the adaptive multilevel splitting*, presented at the Minisymposium Advances in Monte Carlo Methods and Applications at the ICIAM – Valencia (Spain), July 15–19, 2019

5. **Laura Lopes**, Christophe Chipot, Tony Lelièvre, *Adaptive Multilevel Splitting method: isomerization of the alanine dipeptide*, presented at the Hands–on Workshop on Enhanced Sampling and Free–Energy Calculation – Urbana (IL–USA), September 25–29, 2017