

# Laura Joana Silva Lopes

**Name in bibliographic references** LOPES, L. J. S. or LOPES, LAURA J. S.

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## Post-doctoral Fellow at Los Alamos National Laboratory

### Skills

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**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

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**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 (2<sup>nd</sup> year) Analysis, Modeling and Simulation** Paris–Saclay University

**2014–2015 MSc (1<sup>st</sup> 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

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### Research

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

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

**Supervisor** Danny Perez

**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 2<sup>nd</sup> 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

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### Peer reviewed

- 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 (**accepted**)
- 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 (**accepted**)
- 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**
- 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, v.116, p.2244 – 2260, **2012**
- 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 Fe<sub>2</sub>O<sub>3</sub> and Cu, Cr–Fe<sub>2</sub>O<sub>3</sub> 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

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### 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, *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
2. **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
3. **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
4. **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