Mayk Caldas Ramos | PhD.

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Professional Experience

- **Postdoctoral associate** **Rochester, NY - USA**
  White lab - University of Rochester *2022–Present*
  As a postdoctoral researcher, I have led AI-driven chemistry projects, developing and using RNNs, LLMs, and language agents to predict molecule properties and natural language descriptions of experiment outcomes. Additionally, I have advised and mentored students, guiding them in their research and development. This role has enhanced my expertise in AI and chemistry, as well as my leadership, organizational, and communication skills.

- **Software engineer - Intern** **Rio de Janeiro - Brazil**
  Laboratório de Metrologia Dimensional e Computacional *2021–2022*
  I worked on a team developing software to host a machine-learning model for predicting the presence of oil in high-depth basins given pressure pulse gas gun scans. I had the opportunity to work in a large team and learn how to develop software collaboratively.

- **Graduate researcher** **Rio de Janeiro - Brazil**
  Laboratório de Modelagem Molecular (LabMMol) - UFRJ *2017–2022*
  During my time on LabMMol, I worked applying advanced molecular dynamics (MD) techniques to study biomolecular systems. In addition, I helped to develop a software to build topologies for MD simulations

- **CFD Engineer - Intern** **Rio de Janeiro - Brazil**
  WIKKI Brasil *2016–2017*
  I joined the Wikki team when the company was in its start-up phase. Even as an intern, I worked on real client projects. Because of the complex environment of a start-up, I had multiple attributions. Some of those attributions were consulting, training, designing the company website, and leading the hiring process of a web dev.

- **Undergraduate Researcher** **Rio de Janeiro - Brazil**
  Applied Thermodynamics and Molecular Simulation (ATOMS) - UFRJ *2015–2017*
  As an undergrad student, I had my first contact with molecular dynamics (MD) simulation by applying this method in gas phase separation systems. I proposed the project I started working on. Applying MD to simulate zeolites became an active research line of the laboratory after I initiated it.

Awards and prizes

- Octávio Augusto Ceva Antunes award for academic excellence
- First place on the LLM in Materials and Chemistry March Madness Hackathon 2023
- Top15 on the University of Rochester Biomedical Data Science Hackathon Summer 2022

Education

Academic Qualifications

- **Federal University of Rio de Janeiro (UFRJ)** — **Rio de Janeiro - Brazil**
  PhD in Chemical Sciences — *2019–2022*
  Thesis: Evaluation of the viability of PAMAM dendrimer in their use as drug carriers by molecular dynamics.

- **Fluminense Federal University (UFF) - CEDERJ** — **Niterói - Brazil**
  Bachelor in Computing Systems — *2020–2022*
  Thesis: QScrapper2.0: web scraping HIV medicine data from Quora

- **Federal University of Rio de Janeiro (UFRJ)** — **Rio de Janeiro - Brazil**
  Masters in Chemical Sciences — *2017–2019*
  Thesis: Molecular dynamics simulations of PAMAM and PPI dendrimers using the GROMOS-compatible 2016H66 forcefield: structural properties for different generations and pH environments.

- **Federal University of Rio de Janeiro (UFRJ)** — **Rio de Janeiro - Brazil**
  Bachelor of Chemical Engineering — *2012–2017*
  Thesis: A molecular dynamics study of water diffusion in LTA-type zeolites.

Publications

- Jablonka, Kevin Maik; et al. (Aug. 2023). **"14 examples of how LLMs can transform materials science and chemistry: a reflection on a large language model hackathon"**, Digital Discovery. issn: 2635-098X. doi: 10.1039/D3DD00113J. url: https://pubs.rsc.org/en/content/articlelanding/2023/DD/D3DD00113J.
- **Ramos, Mayk Caldas** and Andrew D White (July 2023). **"Predicting small molecules solubilities on endpoint devices using deep ensemble neural networks"**, arXiv:2307.05318 [physics.chem-ph]. url: https://arxiv.org/abs/2307.05318.
- **Ramos, Mayk Caldas**; et al. (Apr. 2023). **"Bayesian Optimization of Catalysts With In-context Learning"**, arXiv: 2304.05341 [physics.chem-ph]. url: http://arxiv.org/abs/2304.05341.
- **Ramos, Mayk C.** and Horta, Bruno A. C. (Feb. 2021). **"Drug-Loading Capacity of PAMAM Dendrimers Encapsulating Quercetin Molecules: A Molecular Dynamics Study with the 2016H66 Force Field"**, J. Chem. Inf. Model. 61.2, pp. 987–1000. issn: 1549-9596, 1549-960X. doi: 10.1021/acs.jcim.0c00960. url: http://dx.doi.org/10.1021/acs.jcim.0c00960.
- **Ramos, Mayk C.**; et al. (Apr. 2021). **"pyPolyBuilder: Automated Preparation of Molecular Topologies and Initial Configurations for Molecular Dynamics Simulations of Arbitrary Supramolecules"**, J. Chem. Inf. Model. 61.4, pp. 1539–1544. issn: 1549-9596, 1549-960X. doi: 10.1021/acs.jcim.0c01438. url: http://dx.doi.org/10.1021/acs.jcim.0c01438.
- **Ramos, Mayk C.**, Horta, Vitor A. C., and Horta, Bruno A. C. (Apr. 2019). **"Molecular Dynamics Simulations of PAMAM and PPI Dendrimers Using the GROMOS-Compatible 2016H66 Force Field"**, J. Chem. Inf. Model. 59.4, pp. 1444–1457. issn: 1549-9596, 1549-960X. doi: 10.1021/acs.jcim.8b00911. url: http://dx.doi.org/10.1021/acs.jcim.8b00911.

Interests and Objectives

- **Large Language Model-based tools**
  To translate chemistry for a natural language framework aiming to leverage large language models using both structured and unstructured scientific data
- **Data-driven Science and Software Development**
  Developing tools in the context of inverse molecular design applying machine learning and computer vision in chemistry.
- **Molecular Modelling and Simulation**
  To study systems of interest using simulation softwares and techniques aiming to understand biomolecular systems better
- **Simulation Techniques**
  To develop and implement new simulation techniques and create scripts for automating simulation processes

Technical and Personal skills

- **Programming Languages:**
  - Proficient in: Python, Bash scripting, LaTeX
  - Familiar with: Fortran90, C, C++, JavaScript
- **Known Scientific Softwares and libraries:**
  - pyTorch, tensorflow, HuggingFace, openAI, scikit-learn
  - Molecular Dynamics: GROMACS, Lammps, VMD, pyMol
- **Languages:** Portuguese (Native), English (Fluent).
- **General Business Skills:** Good presentation skills, Works well in a team, Linux administration, Notion management, collaborative development with git/github.

Talks and posters

- **Geothermal AInnovation Competition** **(Online) - USA**
  Event kick-off seminar *2023*
  Title: How Large Language Models are Impacting Chemistry
- **Platform for Advanced Scientific Computing Conference (Online) - Davos - Switzerland**
  Minisymposium Presentation *2023*
  Title: Using In-Context Learning and Frozen Large Language Models for Bayesian Optimization of Catalysts
- **APS/ICTP-SAIFR** **Rio de Janeiro - Brazil**
  Poster presentation *2020*
  Title: Using multiple-restrained molecular dynamics to evaluate the loading capacity of quercetin molecules in PAMAM dendrimer
- **XX Brazilian Symposium on Theoretical Chemistry** **Rio de Janeiro - Brazil**
  Poster and Oral presentations *2019*
  Title: Using steered molecular dynamics simulations for building models of dendrimer-drug complexes
- **Molecular Modeling in Biological Systems School** **Rio de Janeiro - Brazil**
  Poster and Oral presentations *2018*
  Title: Molecular Dynamics of PAMAM and PPI dendrimers using GROMOS-compatible 2016H66: Systematic analysis of pH and generation effects