Celso Rêgo

nationality: Brazilian
born 1981 (Santarém-Pa)
Karlsruhe, Germany

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Education

2017 **Ph.D. Physics (Theory)**
IFSC, São Carlos – Brazil

2012 **M. Sc. Physics**
UFAM, Manaus – Brazil

2010 **B. Sc. Physics**
UFAM, Manaus – Brazil

Languages

Portuguese	native
English	●●●●●
Spanish	●●●●○
German (B1)	●●●○○

Programming

Python	●●●●●
Fortran	●●●●●
MatLab	●●●●○
Bash	●●●●○
HTML	●●●◐○
CSS	●●●○○
C++	●●●○○
Git and Docker	●●●●○

(*)[The language and programming scales are from 0 (Fundamental Awareness) to 5 (Expert).]

Software and tools

- Office: Word, Powerpoint, Excel, LaTeX, GIMP, Kdenlive
- Linux (advanced), Windows
- High-Performance Computing
- Functional and Object-Oriented Programming

Experience

Since 2023, I have coordinated the ScienceAI initiative at the Karlsruhe Institute of Technology (KIT), integrating predictive and generative AI with theoretical chemistry and chemical data science. My research advances eco-friendly materials by combining multiscale modeling with FAIR, workflow-driven knowledge graphs, addressing critical challenges in protein folding, nanocatalysis, next-generation batteries, two-dimensional semiconductors, and solar-cell materials. From October 2022 to May 2024, the Platform MaterialDigital consortium entrusted me with the CEO role of the Matmatch industrial materials platform, enabling me to bridge experimental and theoretical science with industrial demand and societal value. I now serve as Principal Investigator of the HelmholtzAI-funded GENIUS project, further expanding the translational impact of AI-driven materials discovery. Throughout my career, I have mentored Ph.D. candidates and Postdocs, guiding their work toward publication in premier scientific journals, presentation on global stages, and tangible R&D outcomes.

since Jan 2020 **Senior-Scientist**
Karlsruhe Institute of Technology
https://www.int.kit.edu/1632_5881.php
https://www.materialdigital.de/workflows
https://big-map.github.io/big-map-registry/

Development of workflows as digital twins within the MaterialDigital and Battery2030+ projects.

May. 2017 – Oct. 2019. **Postdoctoral researcher**

Max-Planck Institute for Microstructure Physics Halle, Germany
Method development to study atoms scattering on metallic surfaces.

Mar. 2013 – Nov. 2017. **Ph.D. student**

Institute of Physics of São Carlos, Brazil
Computational Chemistry study of Molecules on Surfaces.

Selected achievements

40+ scientific publications, talks and conferences contributions.
https://scholar.google.de/citations?hl=de&user=LF6dHGsAAAAJ

Played the CEO role of Matmatch from October 2022 to May 2024.

Proposer & Coordinator of **ScienceAI** initiative
https://scienceai.int.kit.edu/
(only at KIT)

Developer of the SimStack workflow framework.
https://simstack.readthedocs.io/en/latest/

GENIUS: Generating Efficient Multiscale Simulation Protocols Using ScienceAI
https://github.com/KIT-Workflows/agentic-workflow-framework

Awarded in 2014 with the Yvonne Primerano Mascarenhas prize. 1st place at SIFSC IV conference (Ph.D. student category).
https://www2.ifsc.usp.br/portal-ifsc/iv-sifsc/

Skills

Multiscale Modeling and Digital Transformation:

- User of more than ten modeling codes covering different methods such as **Density Functional Theory, Molecular Dynamics, Monte Carlo, Finite Element Method, Continuous Model, Computational Chemistry, and Predictive** & **Generative AI**.
- Boosting scientific collaborations (Theory and Experiment).

Management:

- Bitrix24, Mattermost, Rocket.Chat, Slack, and Miro.

Personal:

- Self-directed learner with a creative and interdisciplinary approach.
- Startup entrepreneurial mindset.
- Team player with intercultural experience.

Last updated: June, 2025.