

# Computational Chemist & Cheminformatics Scientist

## あなたの仕事内容

### Key Targets of the Job:

- Develop and optimize computational workflows integrating quantum simulations, molecular descriptors, and predictive machine learning models
- Apply advanced cheminformatics and data-driven approaches for virtual screening, property prediction, and reaction mechanism analysis
- Design and implement automated pipelines for high-throughput quantum chemical calculations and machine learning model training
- Model and simulate complex chemical reaction mechanisms across diverse environments using quantum mechanical and ML-assisted approaches
- Analyze simulation results to extract molecular-level insights and support experimental design or product development
- Conduct comprehensive literature reviews and generate high-quality technical documentation, reports, and presentations
- Collaborate effectively within an interdisciplinary team of computational scientists, chemists, physicists, and materials engineers
- Support external collaborations, joint research projects, and technology scouting initiatives
- Demonstrate a willingness to travel occasionally for project meetings, conferences, and collaborative activities

## あなたのプロフィール

- PhD in quantum chemistry, computational chemistry, cheminformatics, materials science, physics, or a closely related field (mandatory academic background)
- Proven hands-on experience with quantum chemistry methods (e.g., DFT, ab initio) and related software (e.g., Gaussian, ORCA, VASP, CP2K, DMol<sup>3</sup>)
- Strong background in cheminformatics, including experience with molecular representations and libraries such as RDKit and Open Babel
- Demonstrated ability to incorporate machine learning (e.g., scikit-learn, PyTorch, TensorFlow) into computational chemistry workflows
- Experience in modeling reaction mechanisms, energy landscapes, or catalytic processes at the atomic or molecular level - good to have
- Proficiency in Python (preferred), along with experience using scientific computing libraries such as NumPy, pandas, and ASE
- Familiarity with molecular dynamics tools (e.g., GROMACS, LAMMPS) is a plus
- Postdoctoral or several years of industrial experience in the field is highly preferred
- Excellent written and spoken English communication skills, with the ability to articulate complex technical concepts to diverse audiences



ジョブID

**REF860000**

業務分野

研究開発

勤務地

**Lousado**

リーダーシップレベル

**Leading Self**

勤務に関する柔軟性

**Onsite Job**

法的事項

**Continental Mabor Indústria de Pneus S.A.**

- Strong analytical thinking, creativity, and a proactive, solution-oriented approach to problem solving
- Ability to work independently and collaboratively within cross-functional and interdisciplinary teams
- Portuguese languages skills written and spoken is a plus

## オファー

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## 会社概要

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