Computational Chemist & Cheminformatics Scientist

工作职责

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

职位要求

- 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, DMol³)
- 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

职位号码
REF86000O

工作职能
研发

所在地
Lousado

领导力级别
个人贡献者

工作场所灵活度
现场办公

法律实体名称
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

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