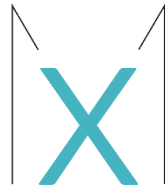# R&D Engineer

Matgenix

Who We Are

Matgenix is an innovative and dynamic company founded in 2020, located in Belgium at the south of Brussels. At Matgenix, we use cutting-edge methods and technologies in materials simulation, data management, data consolidation and machine-learning techniques for industries active in chemistry and materials. We develop tools and software to accelerate the search, design and optimization of new materials, compounds, and processes.

Our Purpose

Empower our partners and customers to create sustainable and resilient applications through innovative material design, shaping a better future for generations to come.

Our Vision

Position ourselves as the forefront of material discovery through virtual screening, pushing boundaries and revolutionary advancements across industries and sustainability initiatives.

Our Team

We are a team of enthusiastic and passionate experts in materials science and chemistry.

We are looking for an R&D Engineer (M/F) with experience in molecular simulations of materials, molecules and compounds, with experience in machine-learning applied to chemistry and materials, and with a strong background in programming.

About You

Your Experience

Essentials

- You have a PhD in computational materials science, computational chemistry or related field.
- You have expertise in computational modeling of materials, molecules, reactions, and/or processes at the atomistic level.
- You have experience with molecular dynamics simulation packages (e.g., Lammps, Gromacs, …) and/or with density functional theory software (e.g. Abinit, QuantumEspresso, Vasp, Turbomole, Gaussian, …).
- You have expertise in machine learning techniques and have knowledge of the most standard tools for machine learning (e.g., Scikit-Learn, TensorFlow, Pytorch, …).

- You can demonstrate excellent coding skills in Python.
- You are familiar with good software development practices.
- You are familiar with Unix/Linux systems and with executing simulations on large supercomputers.
- You are self-motivated, team player, hands on, autonomous, rigorous and flexible. You are able to quickly learn about new topics.
- You have good communication skills (oral and written) in English.

Nice to have
- You have experience in working with industry.
- You have expertise in the usage or development of automated workflow for simulations (e.g., using Atomate2/jobflow/Fireworks/Atomate, ASE/ASR, Aiida, …).
- You have expertise, knowledge and/or experience in DevOps.
- You have expertise and/or experience in front-end development, full-stack development.

Your roles
- You interact with international industrial customers from all over the world.
- You effectively communicate with technical and non-technical stakeholders.
- You execute and manage projects with industrial or academic collaborators.
- You collaborate closely with team members and external partners to ensure project success.
- You develop and run simulations for various systems, ranging from molecules to surfaces and bulk systems.
- You write scientific and technical specifications for proposals.
- You develop automated tools to optimize our internal processes and you support the design and development of interfaces (e.g., web app) for users and customers.

Benefits
- You work in a young and innovative start-up located at the heart of Europe. You join a human scale and dynamic company with a motivated team.
- You work in close collaboration with highly skilled partners and customers, in an enriching ecosystem of tech and digital innovation.
- You work on interdisciplinary domains, e.g., energy, transport, aerospace, metallurgy, …
- You constantly acquire new skills and broaden your competences by learning or developing cutting-edge methods, tools and technologies.
- You get a competitive and flexible salary package with attractive benefits.
- You can enjoy flexible working arrangements, including the possibility of remote or home-based work, allowing for a healthy work-life balance tailored to your needs.

How to apply
This position will remain open until filled. However, regardless of application status, all candidates can expect to receive initial feedback by 22nd May 2024.

Send your application to jobs@matgenix.com. Your application should include:

- CV with your research experience, list of publications and projects
- Examples of your coding in python packages (e.g. github/gitlab links)
- At least two references (name and e-mail)