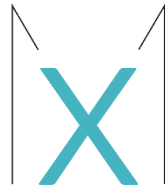


# R&D Engineer



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 at 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., Lammmps, 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 22<sup>nd</sup> May 2024.

Send your application to [jobs@matgenix.com](mailto: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)