

# COMPUTATIONAL MATERIALS SCIENTIST

#### THE COMPANY

EmTDLab is a company founded in 2018 with the vision to advance the future of space exploration.

Effective shielding against space radiation represents one of the most challenging concerns of space missions, from satellite on-board systems to deep space human flight. Our goal is to participate in the discovery of entirely new materials for space radiation shielding. Our engineering services and product will soon complement the technologies deployed by the largest and most ambitious aerospace companies.

To do so, EmTDLab has developed a novel proprietary method to identify new advanced materials with optimal radiation shielding parameters and mechanical properties. Based on the support of the European Space Agency, EmTDLab aims to actively develop the technology to synthetize and manufacture those materials with optimal properties.

#### THE POSITION

EmTDLab is growing and actively recruiting a computational materials scientist. We are looking for a creative, self-starting individual who will contribute to computational materials discovery in relation to space radiation shielding.

As a key member of the R&D team, you will be responsible for analysing materials science issues from the atomistic perspective and developing artificial intelligence algorithms for materials discovery and properties optimisation.

Candidates are expected to have significant experience in the fields of computational chemistry, material science, and/or materials engineering, and a keen interest in artificial intelligence. They should feel at ease to work with a multi-disciplinary team that includes materials scientists, software programmers, spacecraft systems engineer and radiation engineers.

## WHAT WE OFFER

EmTDLab is a freshly incorporated company in Luxembourg. You will be a key member of a new team with opportunities to have a direct influence in shaping the future of the company. Your opinion matters. EmTDLab is a no-nonsense company with a highly systematic approach to research, development and engineering.

EmTDLab promotes a work culture driven by technical excellence, transparency, integrity, respect, and humour. We encourage diversity in backgrounds. Your appetite for creativity, innovation, intellectual curiosity will be satisfied on a daily basis. Being convinced that cross-functional collaboration is a key success factor, the human capital development policy is not to assign you in fixed roles but to encourage personal development.



EmTDLab is committed to flexible organisational principles with respect to work location, working hours and contractual agreements (e.g. part-time work and full time work). Each team member is expected to fulfil her/his objectives as a part of the company's goals, respecting common sense business logic, commonly agreed research practices, quality assurance and quality control.

We offer a competitive remuneration package in line with the market, including yearly bonuses and training opportunities.

The main place of work (headquarters) is the Grand Duchy of Luxembourg.

Candidates from any third-country national (a person who is not an EEA national – i.e. from an EU Member State, Iceland, Norway and Liechtenstein – or a Swiss Confederation national) space are encouraged to apply under a residency permit application.

#### **RESPONSIBILITIES**

Your responsibilities as a Computational Materials Scientist at EmTDLab may include:

- Perform and analyse computational chemistry simulations, e.g. to predict materials properties
- Implement machine learning algorithms for the prediction of materials properties
- Formulation of development objectives
- Interact with the rest of the team to connect the materials properties microservice with the rest of the EmTDLab software (radiation shielding simulation, mesoscale modelling, etc.)
- Agile software engineering documentation

## **REQUIREMENTS**

#### **Profile**

- Ph.D. in chemistry, physics, material science, or related discipline. MSc candidates may be considered should they demonstrate an excellent profile within the fields described below
- Documented experience in computational chemistry and/or programming and/or machine learning
- Experience in working in industry R&D is considered as an advantage
- Fluent in spoken and written English; knowledge of other languages is considered as an asset.

### Skills

The ideal candidate should have the hard skills listed below. However, we encourage applications also from those individuals who do not meet each of those requirements.

- Experience with software for quantum chemistry such as VASP, Quantum Espresso, cp2k, etc., ideally documented by scientific publications
- Programming experience, ideally in Python
- Experience in implementing machine learning algorithms
- Excellent knowledge of physics of materials and thermodynamics



In addition, we expect applicants to have the following soft skills:

- A desire to learn and innovate
- Ability to communicate, collaborate, and deliver results as a member of multi-disciplinary teams
- Excellent written and verbal communication skills with recent publications and/or presentations
- Superior organizational and analytical skills with keen attention to detail and quality;

## **APPLICATION PROCESS**

Please send an up-to-date resume to <u>jointheteam@emtdlab.com</u> coupled with a short introduction letter answering the question why our key company approach is important in this role.

The name of at least two references (MSc-PhD supervisors/current employers),

Diploma & copies of educational certificates will be asked during the process

Additional publications, non-confidential papers and previous technical use cases are welcomed and will be considered in the evaluation process.

A short-list of candidates will be made, who will be contacted for a first interview over videoconferencing.

Three rounds of interview will take place in total either through videoconferencing or face-to-face.

It is the policy of EmTDLab to provide equal employment opportunity without regard to race, colour, religion, age, national origin, sex, gender, sexual orientation, gender identity/expression, disability, health status, genetic information, or any other basis, protected by data privacy, institutional policy or by state or local laws unless such distinction is required by law.