COMPUTATIONAL MATERIALS ENGINEER

THE COMPANY

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

Effective shielding against space radiation remains one of the most challenging concern 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 engineer. As a key member of the R&D team, you will be responsible for developing artificial intelligence algorithms for materials chemical composition discovery and optimisation.

Candidates are expected to have significant work experience in the fields of computational chemistry and material science, engineering materials design, and deep understanding of related fields. The ideal candidate will have a keen interest in making major progress in engineering application development with AI technology.

We are looking for a creative, self-starting computational scientist/engineer motivated to contribute to computational materials discovery and co-develop new materials systems for space radiation shielding.

As a team member, developing your own internal and external networks remains crucial. The candidate should feel at ease to initiate and cultivate dynamic collaboration with multi-disciplinary team members including, among others, materials scientists, software programmers, mission scientists, 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.

We work according to flexible organisational principles with respect to work location, working hours and contractual agreements (e.g. part-time work and full time work). We expect that each team member fulfils her/ his objectives as a part of the company's objective with little constraint added to your R&D and engineering work.

We although expect that we all work as professionals and all respect common sense business logic, commonly agreed research practices, quality assurance and quality control. We are an open door policy company where team communication is considered as critical for success.

We offer a 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. The present job offering also covers provisional recruitment for the Kingdom of Belgium.

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.

SCOPE OF RESPONSIBILITIES

- Formulation of development objectives
- Research and benchmarking of existing computational chemistry models and codes
- Mathematical models and algorithms architecture
- Genetic algorithms, machine learning, multi-objective optimisation
- Database design and data collection
- Computational procedures, sensitivity analysis, data visualisation
- Agile software engineering documentation

DESCRIPTION OF RESPONSIBILITIES

Key responsibilities will include:

Define and implement project plans, manage milestones, and hold reviews to assure reliability of projects plan. Both projects and sub-projects will be assigned based on technical steps and work packages.

The computational search for new 2D/3D materials by numerical and geometric simulations.

Design and optimization of engineering materials candidates having optimal radiation shielding parameters and optimal mechanical properties, using advanced computational techniques.

Development and use of high throughput screening codes for the exploitation of material structure related databases and/or artificial intelligence based methods;

Advance internal modelling capabilities (composition and microstructure) through design and implementation of new methodology. Benchmark and document choice of methodologies.

Enable a design-driven and predict-first approach within the team and with external collaborations such as thermodynamics calculation team and microstructure characterization team.

You will support ongoing internal efforts in identifying conceptual and methodological gaps that require to be fulfilled to develop these workflows, and propose innovative solutions to move forward.

You bring advanced dynamic simulations of complex materials into the big picture by supporting the development of bottom-up modelling workflows which combine low-level and high-level methodologies to bridge time- and length-scales.

Furthermore, you play a key role in implementing and supporting a state-of-the-art infrastructure for materials development. Make recommendations for design, process improvements, and data collection; Provide continuous agile software engineering support and documentation.

You have demonstrated experience with modelling of specific engineering materials microstructure components and in particular the impact of the microstructure features (geometric information) on material properties.

Based on high-level problem descriptions you define hypotheses on underlying mechanisms governing the behaviours observed from experimental measurements, set up elaborate models to verify the validity of such hypotheses, provide fundamental understanding and translate the results of the simulations into models (analytical, stochastic) that can be used to describe the behaviour of the system at the material microstructure level, thereby suggesting design rules to improve future materials and product performance.

Establish both in silico and in-situ testing protocols of materials with third parties; elaborate the project management process (including scope, resources, timing and quality assurance) for both materials simulation/modelling and testing protocols.

Write verification test plans, test procedures, and test reports against product requirements; Perform root-cause analysis of test failures and communicate recommended actions;

The scope and description of responsibilities will evolves according to the internal process and product development lifecycle.

REQUIREMENTS

Profile

Ph.D./M.Sc. in chemistry, physics, material science, or related discipline, with a computational emphasis; Post-Doc profile can be considered based on interests and motivation;

Evidence of creative application of computational approaches to problems of engineering materials with optimized chemical and mechanical properties

Fluent in spoken and written English; knowledge of other languages is considered as an asset.

Interpersonal skills and experience

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;

Engineering-related laboratory experience; Experience working in teams of programmers.

Experience / Seniority

0+ years of industry experience with a Ph.D., or 4+ years with a M.S.

Industry related experience in the field of computational materials discovery; including all aspects of molecular design simulation, density functional theory and molecular dynamics;

Experience can be minimal but with a proven track record of fast learning; or experience can be higher such as 4 to 5 years of relevant work experience in the industrial field;

Knowledge and skills

Strong physics, mathematics and statistics knowledge base;

Proficiency in general molecular modelling techniques;

Deep understanding of density functional theory;

Hands-on Computational experience in programming languages including R, Python, Matlab, C/C++, and SQL; R, preferably in a HPC environment;

Experience with genetic algorithms, artificial neural networks, machine learning, and deep learning;

Experience with agile software development engineering requirements / systems engineering documentation.

Track record of original scientific publications and conference contributions.

OPTIONAL ADDITIONAL SKILLS AND EXPERIENCE:

In-depth practice with density functional theory methodologies (VASP, CRYSTAL, QE...) and potential energy surface calculations; energy calculation in a HPC environment using machine learning approaches and/or numerical approximations, analytical equations driven predictions

Theoretical knowledge of computational homogenization

Knowledge in crystallography, microstructure characterization

APPLICATION PROCESS

Please send an up-to-date resume to jointheteam@emtdlab.com 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.