THREE OPEN POSITIONS (THEOS, EPFL, SWITZERLAND) IN COMPUTATIONAL MATERIALS RESEARCH SOFTWARE ENGINEERING

Three positions for research software engineers/computational materials scientists are available in the group of Prof. Nicola Marzari at EPFL in Lausanne, Switzerland, under the supervision of Dr. Giovanni Pizzi.

Outstanding candidates are sought with a **background in the physical sciences** alongside **strong programming skills**. Candidates are expected to show excellent work ethics and to feel at home working in teams both within THEOS and between research groups.

Please also note the four other open positions in computational materials research to be advertised soon at **http://theossrv1.epfl.ch/Main/Openings**

POSITION 1

HIGH-PERFORMANCE COMPUTING, HIGH-THROUGHPUT COMPUTING AND DATA ANALYTICS WITH THE AiiDA MATERIALS INFORMATICS PLATFORM

AiiDA (http://aiida.net) is an open-source python framework for workflow management and provenance tracking in computational materials science. While most core developers are based at EPFL, AiiDA and AiiDA plugins are used and developed in several countries across Europe, both at universities, research institutes and companies. By virtue of its general design and flexible plugin system, AiiDA is easily extended to new codes and new use cases and is already interfaced to almost 60 different materials science codes (see full list on the AiiDA plugin registry). This position provides the opportunity to join an international team of developers in building and sharpening the tools for the computational materials science of the future.

This position is funded by the European Centre of Excellence MaX "Materials design at the Exascale" (http://www.max-centre.eu), where the EPFL MaX team (involving two other researchers) will lead the workpackage "Convergence of high-performance computing, high-throughput computing and high-performance data analytics". The successful candidate will be involved in implementing new features driven by an increasing user base, including object-store integration, advanced sharing capabilities, seamless integration with novel REST-based interfaces available at high-performance computing (HPC) centres. Increasing compute power enables more and larger calculations to be performed, and the candidate will identify and remove bottlenecks when dealing with tens of millions of data entries and thousands of concurrent simulations/workflows. Finally, as part of the core developer team, the candidate will be involved in code maintenance and releases, user support, and AiiDA deployment using various technologies (PYPI, conda, docker, virtual machines via ansible, …).

The contract is initially for 1 year as required by EPFL, and renewable yearly upon mutual satisfaction. Funding from the European MaX Centre of Exellence is available for 3 years, but the contract may be extended to up to 4 years depending on future funding decisions. Level of employment will be 100% on the standard EPFL paygrade (for instance, a gross salary of 81'900CHF/year for a recently-graduated PhD).

POSITIONS 2 & 3

MATERIALS CLOUD: FROM PROTOTYPE TO PRODUCTION AT SCALE

Materials Cloud (http://materialscloud.org) is a web platform designed to enable seamless sharing of resources in computational materials science. This includes educational materials, interactive tools, virtual hardware and, powered by AiiDA, the full provenance of materials science calculations (think of AiiDA as git and Materials Cloud as GitHub). Through its rich web interface, users can run complex calculations and browse their provenance without domain expertise, while maintaining fine-grained access to the underlying workflows and data. Today, the core infrastructure of Materials Cloud is up and running but its official launch dates back only one year. Candidates will join the team of Materials Cloud developers and have the opportunity to shape both features and content of the platform as it scales up. Materials Cloud started as the dissemination platform of the pan-Swiss materials consortium MARVEL, a 12-year federal initiative created in 2014 with the aim of accelerating materials' design and discovery, and is now supported also by the European H2020 MaX Centre of Excellence.

These two positions are funded by a new project sponsored by the swissuniversities P-5 program. Successful candidates will adapt Materials Cloud to meet the needs of research groups in computational materials science (visualizations, plugins, data management plans …), branching out to related fields (e.g. computational physics, computational chemistry). Candidates will expand the services available to the scientific community as a whole (like the Materials Cloud ARCHIVE) through implementing autoscaling solutions that support dynamic workloads and ensure high availability. Finally, candidates will contribute to the maintenance of the automated deployment and monitoring infrastructure of Materials Cloud.

The contract is initially for 1 year as required by EPFL, and renewable yearly upon mutual satisfaction. Level of employment will be 100% on the standard EPFL paygrade (see details in position 1). Funding from swissuniversities is available for 2 years, but the contract may be extended up to 4 years depending on future funding decisions.

SELECTION CRITERIA

Requirements:

- A **background in the physical sciences (physics, chemistry, and materials science/engineering)**. Candidates with a different academic background who can nevertheless demonstrate experience in the physical sciences are also encouraged to apply
- Advanced knowledge of Python
- Familiarity with version control systems (git), issue trackers and writing unit tests
- Web development experience (HTML5, CSS, JavaScript) for the Materials Cloud positions
- Strong organisational skills, including the ability to work independently, to assess priorities and to manage projects involving multiple partners

Desirable skills:

- A PhD in the domain is valuable (but not required)
- Knowledge of software architecture and design (architecture patterns, UML, …)
- Experience with managing software projects in a team (code review, agile development, …)
- AiiDA position:
    - Experience with python coroutines
    - Experience with database systems (e.g. PostgreSQL)
- Materials Cloud positions:
    - Advanced JavaScript knowledge using frameworks such as AngularJS
- Experience with handling large amounts of data

WORK ENVIRONMENT

Successful candidates will join the group of Nicola Marzari (http://theossrv1.epfl.ch/) at the École Polytechnique Fédérale de Lausanne, located in Switzerland on the shores of Lake Geneva and in close proximity to the Swiss and French Alps. This multidisciplinary group is at the forefront of development and applications of materials simulations, and leads the pan-Swiss materials consortium MARVEL, a 12-year federal initiative created in 2014 whose aim is to accelerate materials' design and discovery. Besides the aforementioned MARVEL, MaX and swissuniversities projects, the group is involved in several international projects, including the H2020 MarketPlace project (https://www.the-marketplace-project.eu), H2020 Intersect, the European Materials Modelling Council (EMMC, http://emmc.info) coordination-and-support action, the simulation services for the NFFA (Nanoscience Foundries and Fine Analysis,
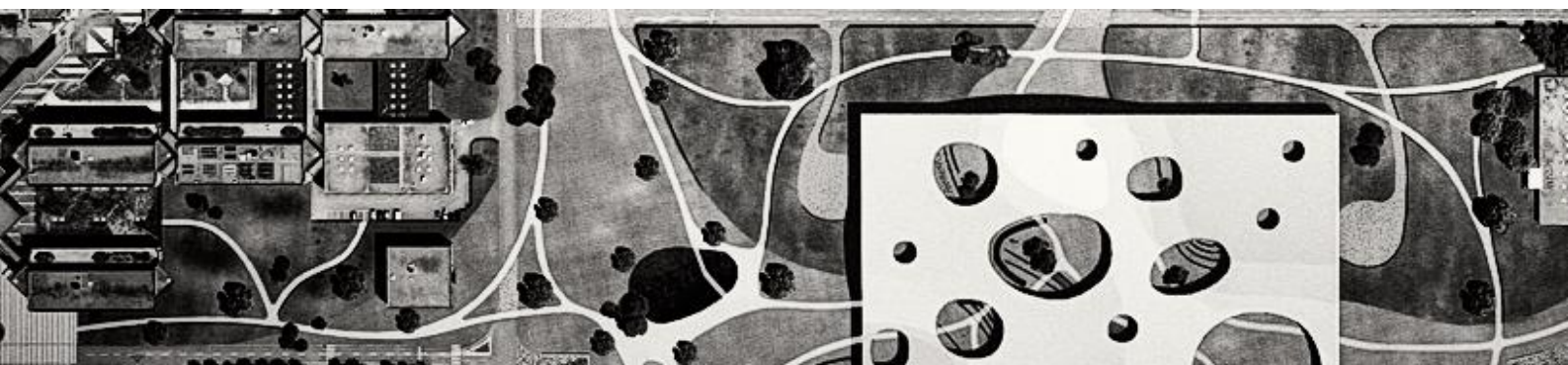
The open positions will involve collecting user feedback and requirements from collaborating groups (which is why a robust scientific background is important) as well as implementing solutions together with the AiiDA and Materials Cloud teams. Candidates should be interested in making state-of-the-art model-ling tools available to diverse communities (students, experimentalists, computational researchers, indus-try), and advancing the integration of AiiDA and Materials Cloud with large-scale efforts like the European Open Science Platform both through software development and by co-organizing tutorials and work-shops. The positions will allow candidates to acquire and strengthen their skills in a number of industry-standard technologies for data management, web development and deployment (databases, SWIFT ob-ject store, REST APIs, visualization frameworks such as d3.js/bokeh/plot.ly dash, docker, ansible, Open-Stack, kubernetes, …).

Upon interest, scientific research projects within THEOS or in collaboration with other research groups involved (e.g. LSMO, C3MP, …) can be incorporated where they align with the objectives of the funding projects.

APPLICATIONS

Candidates should submit two PDF documents: 1) a full CV, including contacts for at least two references and 2) a cover letter of intent (also clarifying which position they are applying for). The documents should be emailed to giovanni.pizzi@epfl.ch and elsa.passaro@epfl.ch (simultaneously; not two emails) with the exact text "AiiDA/Materials Cloud computational materials research software engineer" in the subject line. Shortlisted candidates will be contacted individually for initial interviews, first over Skype video con-ferencing. For best consideration, applications should be submitted by Jan 31st, 2019; the positions will remain open until suitable candidates have been found.