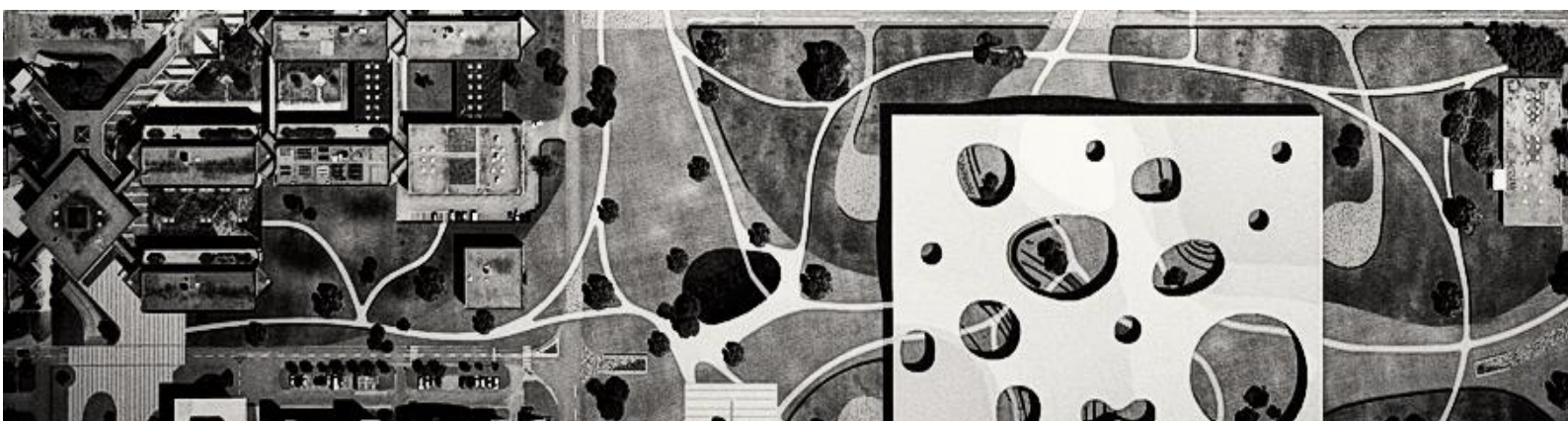# TWO DOCTORAL/POSTDOCTORAL POSITIONS IN: 1) HIGH-THROUGHPUT MATERIALS DISCOVERY, 2) HPC/HTC/HPDA SOFTWARE ENGINEERING THEOS, EPFL, SWITZERLAND

Two doctoral/postdoctoral positions are available in the Laboratory for Theory and Simulation of Materials (http://theossrv1.epfl.ch) at EPFL in Lausanne, Switzerland, under the supervision of Dr. Giovanni Pizzi and Prof. Nicola Marzari. Outstanding candidates are sought with a **strong background in the physical sciences and engineering** alongside **a passion for programming**. Candidates are expected to show excellent work ethics and to feel at home working in teams.

These job openings provide the opportunity to join an exciting and very driven international team at the forefront of research in the field of materials discovery and design, enabled by **AiiDA** (http://aiida.net), an open-source python framework for automated workflow management and provenance tracking. The candidate will join the scientific group at EPFL, collaborating with groups around the world (at universities, research institutes and companies) where AiiDA and its plugins are developed and used to enable the discovery of next-generation materials.

Position 1 – High-throughput materials discovery: The successful candidate will be involved in materials discovery projects that involve the development of new capabilities dedicated to the automated calculation of advanced materials properties. Typical tasks will involve computing novel properties – from thermodynamics to spectroscopies; enabling novel methods; increasing the automation and robustness of the calculations; automatic optimisation of parallelisation parameters to maximise performance of the simulation codes on next-generation exascale architectures.

Position 2 – Convergence of HPC/HTC/HPDA on exascale machines: The successful candidate will be involved in implementing new features in AiiDA, focusing on its scalability towards exascale systems, and in particular on calculation throughput and on unlocking seamless management and analysis of large amounts of interconnected data. Possible tasks will include object-store integration, advanced data sharing capabilities, or improved deduplication of data in the file repository and in the database. This position will involve also code maintenance and releases (for AiiDA core or the AiiDA-Quantum ESPRESSO plugins), AiiDA user support, and deployment using various technologies (PYPI, conda, docker, virtual machines via ansible, …).

The contracts are initially for 1 year, as required by EPFL, and renewable yearly upon mutual satisfaction. Funding is available for at least 2 years, but the contract can be extended for up to 4 years, depending also on future funding. Doctoral appointments are prospectively for 4 years. Level of employment is 100% on the standard EPFL paygrade (for instance, a gross salary of 81'900 CHF/year for a recently-graduated PhD, and 51'400 CHF/year for a starting PhD).

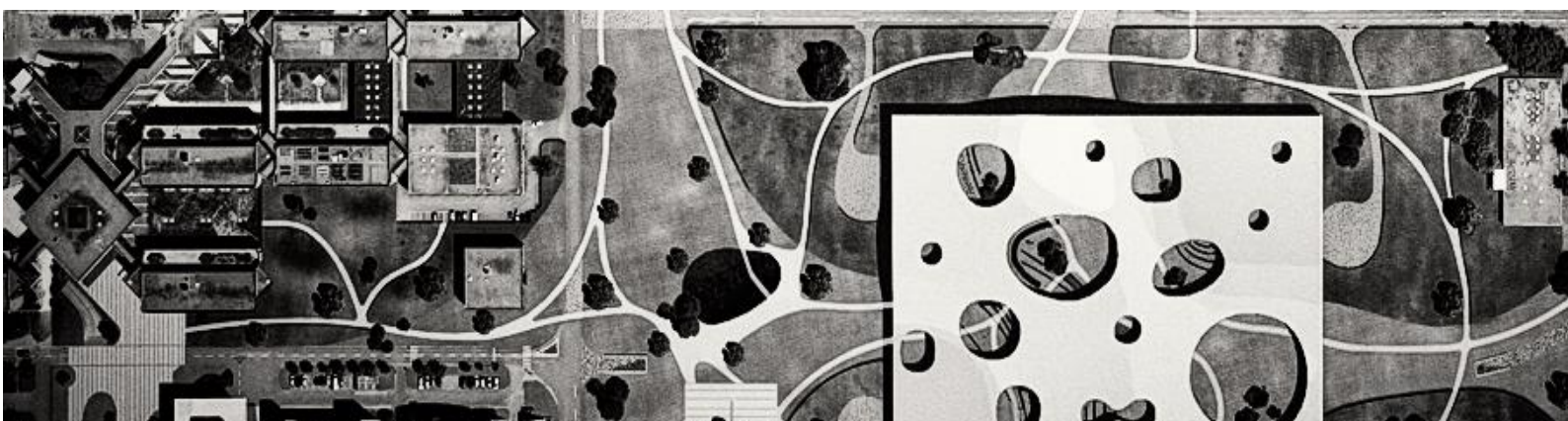# SELECTION CRITERIA

Requirements:

- A **background in physics/chemistry/materials science**. Position 1 requires demonstrated expertise with electronic-structure methods and computational materials science, at the undergraduate level for a doctoral candidate, and at the PhD level for a postdoctoral candidate. Candidates with a different academic background who can nevertheless demonstrate experience in the domains above are also encouraged to apply.
- **Advanced** knowledge of Python (object-oriented programming, class inheritance, …), especially for position 2.
- Dedication to work and strong organisational skills, including the ability to work independently, to assess priorities and to manage projects involving multiple partners.

Desirable skills for Position 2

- A PhD in the domain.
- Knowledge of software architecture and design (architecture patterns, UML, …).
- Experience with managing software projects in a team (code review, agile development, …).
- Experience with: python coroutines; and/or database systems (e.g. PostgreSQL); and/or handling large amounts of data.

FUNDING

The positions are funded by the European Centre of Excellence MaX "Materials design at the Exascale" (http://www.max-centre.eu), where the EPFL MaX team leads the work package "Convergence of high-performance computing, high-throughput computing and high-performance data analytics", and by the Open Science Platform of the Swiss MARVEL NCCR (http://nccr-marvel.ch), dedicated to the promotion

of Open Science and of the technologies that enable it. Both projects support the development and extensive application of AiiDA and of its plugins (over 30 different materials science codes are already interfaced with AiiDA, see full list on the AiiDA plugin registry).

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 and MaX projects, the group is involved in several international projects, including the H2020 MarketPlace project (https://www.the-marketplace-project.eu), the H2020 Intersect project (http://intersect-project.eu), the simulation services for the NFFA (Nanoscience Foundries and Fine Analysis, http://nffa.eu), and the swissuniversities P-5 "Materials Cloud" project (https://www.materialscloud.org/swissuniversities), together with further national, industrial, and computational projects. Outstanding computing facilities are available both on-site and at CSCS (Switzerland) and CINECA (Italy).

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 (clarifying position 1 or 2, and if at the doctoral, postdoctoral, or software scientist level). The documents should be emailed to giovanni.pizzi@epfl.ch, sebastiaan.huber@epfl.ch and nicola.marzari@epfl.ch (simultaneously; not three emails) with the exact text "High-throughput/high-performance materials discovery positions" in the subject line. Shortlisted candidates will be contacted individually for initial interviews, first over Skype video conferencing. For best consideration, applications should be submitted by Nov 24th, 2019; the positions will remain open until suitable candidates have been found.