

## TWO POSTDOCTORAL POSITIONS SPECTRAL PROPERTIES ON ACCELERATED ARCHITECTURES THEOS, EPFL, SWITZERLAND

Two positions for computational physicists/computer scientists are available at the École Polytechnique Fédérale de Lausanne (Lausanne, Switzerland) in the [group of Prof. Nicola Marzari](#). The positions are supported by the [Swiss Platform for Advanced Scientific Computing](#) (PASC) and are renewable yearly; current funding is for 3 years each. If so desired, a possible working location at the Paul Scherrer Institute (Villigen) in the newly created [Laboratory for Materials Simulations](#) may be possible.

The positions will contribute to the development of scientific software to calculate spectral properties of materials on complex accelerated hardware architectures, as deployed in existing HPC systems and in future pre- and exascale machines. The positions will integrate existing implementations of advanced density-functional formulations (Koopman's spectral functionals, extended Hubbard functionals (U/V/J), maximally-localized Wannier functions) with [SIR-IUS](#), a library for electronic structure calculations developed at [Swiss National Supercomputing Centre](#) (CSCS) to provide support to several density-functional theory codes on accelerated architectures.

Outstanding candidates are sought with a strong interest in methodological and software development, and with programming abilities in Fortran and/or C++ and parallel computing, preferably with a background in physics/chemistry/materials or engineering/computer science. A knowledge of the CUDA programming model is a plus.

Close collaborations will take place with the Swiss Supercomputing Center [CSCS](#), and natural synergies will be present with the Swiss National Centre [MARVEL](#) on Computational Design and Discovery of Novel Materials and the H2020 [MaX Centre of Excellence](#) on Materials Design at the eXascale.



## REQUIREMENTS

- **Education**

- A PhD in the physical sciences (physics, chemistry, or materials), engineering, or computer science. Alternatively, a MSc with a proven track record in these domains.
- Basic knowledge of solid-state physics and density-functional theory is a plus.

- **Essential Knowledge and Professional Experience**

- Experience in numerical methods, code development and scientific computing.
- Good knowledge and experience in Fortran and/or especially C++ programming.
- Strong organizational skills, including the ability to manage complex projects involving multiple partners from academia in a highly collaborative environment.
- Passion for HPC computing and programming, and self-motivation for learning.

- **Additional Knowledge and Professional Experience**

- Knowledge of basic parallel programming models (MPI, OpenMP)
- Experience in electronic-structure methods and density-functional theory is an advantage.
- Knowledge of Python.

## FUNDING AND WORK ENVIRONMENT

The successful candidates will join the group of Nicola Marzari (<http://theosrv1.epfl.ch/>) at the École Polytechnique Fédérale de Lausanne (EPFL), located in Switzerland on the shores of Lake Geneva and in close proximity to the Swiss and French Alps. If so desired, a possible working location at the Paul Scherrer Institute (Villigen) in the newly created [Laboratory for Materials Simulations](#) may be possible.



This multidisciplinary group is at the forefront of development and applications of materials simulations, and leads the pan-Swiss materials consortium MARVEL (<http://nccr-marvel.ch>), a 12-year federal initiative created in 2014 whose aim is to accelerate materials' design and discovery. The group is also leading the workpackage on convergence of HPC, high-throughput computing and high-performance data analytics of the H2020 MaX Centre of Excellence (<http://www.max-centre.eu>). The group is actively involved in several international projects, including the H2020 BIG-MAP, MarketPlace, Intersect, OpenModel, DOME 4.0 and NEP/NFFA projects, the swissuniversities P-5 "Materials Cloud" project, together with further national, industrial, and computational projects.

Outstanding computing facilities are available both on-site and at CSCS (Switzerland).

### APPLICATIONS

Candidates should submit 1) a full CV (ideally including BA/MSc transcripts), 2) contact information for two to four references and 3) a cover letter of intent. These documents should be emailed simultaneously to [nicola.marzari@epfl.ch](mailto:nicola.marzari@epfl.ch) and [nicola.colonna@psi.ch](mailto:nicola.colonna@psi.ch) and [iurii.timrov@epfl.ch](mailto:iurii.timrov@epfl.ch) as a single email with one PDF attachment, with the exact text "PASC spectral" in the subject line. Shortlisted candidates will be contacted individually for initial interviews, first via video conferencing.

For best consideration, applications should be submitted by **Oct 31 2021**; the positions will remain open until filled. The contract is renewable every year (as required by EPFL) up to 4 years upon mutual satisfaction and availability of funding; current funding is for 3 years per position. Gross salaries for a freshly minted Ph.D. start at 83'600 CHF/year (~76'500 EUR/year); social benefits (unemployment, pension) are also provided.

