

## FOUR OPEN POSITIONS (THEOS, EPFL, SWITZERLAND) FOR POSTDOCS OR PHDs IN COMPUTATIONAL MATERIALS SCIENCE

Four positions are available at the École Polytechnique Fédérale de Lausanne (EPFL, Lausanne, Switzerland) in the group of Prof. Nicola Marzari – these positions are described below, and would be typically suited to a postdoctoral appointment; appointments at the PhD level would also be appropriate, for candidates with an early (MSc) track record in electronic-structure simulations; one of these would also be suitable for a research software engineer.

Outstanding candidates are sought with a background in the physical sciences (physics, chemistry, materials science, and others field of engineering) or computer science, with passion and commitment to the field, and with a commensurate academic record. Expertise in the development and application of first-principles techniques is required; experience with high-throughput calculations a plus for position 2) and 3), and needed (unless extensive HPC and C++ is shown) for position 4).

- 1) one postdoctoral/PhD position on the development and application of Koopmans' compliant functionals in solids, and further extensions to include dynamical functionals, Bethe-Salpeter integration, or Kadanoff-Baym dynamics
- 2) one postdoctoral/PhD position on equilibrium thermodynamics, defects, and performance of functional materials
- 3) one postdoctoral/PhD position on materials properties on demand (through AiiDA workflows) and materials for neuromorphic computing
- 4) one postdoctoral/software engineer position on high-throughput calculations, and integration and support of Quantum ESPRESSO with SIRIUS (<https://github.com/electronic-structure/SIRIUS>)

**Also note 3 other positions advertised here, dedicated to materials' informatics: <http://theossrv1.epfl.ch/Main/Openings>**

### The environment:

The successful candidates will join the group of Nicola Marzari (<http://theossrv1.epfl.ch/>) at EPFL, 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 in the development and application 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. The group is closely involved in several projects, including the H2020 Max Centre of Excellence for e-Infrastructure in Materials (2015 to 2021), the H2020 MarketPlace project (<https://www.the-marketplace-project.eu>, 2018-22), H2020 Intersect (2019-21), the European Materials Modelling Council (EMMC, <http://emmc.info>), the simulation services for the NFFA (Nanoscience Foundries and Fine Analysis, <http://nffa.eu>), and the Graphene Flagship (<http://graphene-flagship.eu>), together with several other national, industrial, and computational projects, including close collaborations with industry. Outstanding computing facilities are available on-site and at CSCS (Switzerland) and CINECA (Italy).

## **Applications:**

Candidates should submit a single pdf document containing 1) a letter of intent and 2) a full CV, including contacts for at least two references, as an email to [nicola.marzari@epfl.ch](mailto:nicola.marzari@epfl.ch) with the exact text "THEOS Positions" (without inverted commas) in the subject line. Shortlisted candidates will be then contacted individually for initial interviews, first over Skype video conferencing.

For best consideration applications should be submitted by Jan 31<sup>st</sup>, 2019; the positions will remain open until filled. The contracts are for 1 year (as required by EPFL) renewable upon mutual satisfaction, up to 4 years depending on future funding decisions. Starting gross salary for a recently graduated PhD is 81,900 CHF/year (taxes are of the order of 25%); for a starting PhD student 51,400 CHF/year.

