TWO OPEN POSITIONS
BIG-MAP AND MARVEL POSTDOCS/SOFTWARE ENGINEERS
THEOS, EPFL, SWITZERLAND

Two open positions for postdocs/software engineers are available at EPFL (Lausanne, Switzerland), supported by the BATTERY2030+ BIG-MAP project (http://big-map.eu) and the MARVEL NCCR (http://marvel-nccr.ch), within the Laboratory for Theory and Simulation of Materials (http://theossrv1.epfl.ch) at EPFL in Lausanne, Switzerland, under the supervision of Prof. Nicola Marzari and Dr. Giovanni Pizzi.

The goals of the positions are to strengthen the coupling of the Materials Cloud Archive (https://archive.materialscloud.org) with automatic simulations powered by AiiDA (https://www.aiida.net/) and made available as easy-to-use graphical apps in the AiiDAlab portal (https://www.materialscloud.org/aiidalab). The candidates will be thus 1) developing and providing to the community powerful and robust simulation tools, published open source, to predict materials properties (some examples include the prediction of materials properties towards the development of novel batteries, or the simulation of XPS spectra and other computational spectroscopies towards the interpretation of experiments), and/or 2) they will be contributing to make available on the Materials Cloud portal (https://www.materialscloud.org) highly curated and fully open datasets to the whole scientific community (see e.g. the MC3D and MC2D databases of inorganic 3D and 2D crystal structures in the Materials Cloud Discover section: https://www.materialscloud.org/discover).

In addition, the candidates will support and contribute to the development and deployment of the underlying technologies, such as the already mentioned Materials Cloud web portal, the AiiDAlab platform and the underlying AiiDA workflow engine, a materials informatics framework that acts as a flexible and scalable infrastructure to manage high-throughput computations. If desired, scientific research challenges can also be incorporated in the effort.

This job opening provides the opportunity to join an exciting and very driven international team at the forefront of research in the field of materials discovery and design. The candidates will join the scientific group at EPFL, and will be working within a team of 10+ PhD students, postdocs, and software specialists with diverse backgrounds (physicists, chemists, materials scientists, computer scientists) actively contributing to AiiDA, Materials Cloud and AiiDAlab. They will also be collaborating with groups around the world (at universities, research institutes and companies) where AiiDA, its plugins and the Materials Cloud portal are developed and used to enable the discovery of next-generation materials. Furthermore, the position will allow candidates to learn and build strong competences on technological aspects related to scientific software engineering, development and deployment.

SELECTION CRITERIA

Requirements:

- Strong Python programming skills

- Experience in running materials simulations on HPC systems

- Experience in scientific software development

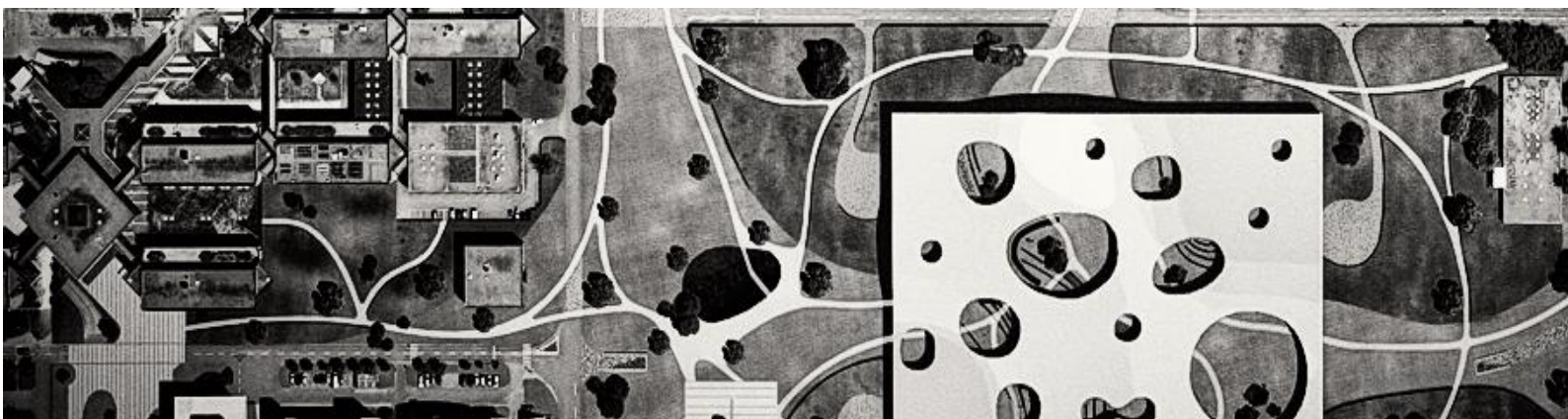- Passion for making software tools open and available to a broad audience of users and researchers

Other desirable (but optional) skills:

- Experience with software to manage high-throughput runs of simulations

- Management of large codes/projects in a team (version control systems, issue trackers, unit testing, continuous integration and other good software practices)

- Experience with REST API (backend) development

- Experience with Docker and with cloud services – e.g. Amazon AWS, Google Cloud Platform, Microsoft Azure, or OpenStack

- Experience with web frontend technologies (HTML, CSS, JavaScript), web/UI frameworks

Outstanding candidates are sought with a **PhD in the physical sciences (e.g. physics, chemistry or materials science/engineering)**, or comparable skills and experience. Candidates are expected to show excellent work ethics and to feel at home working in teams.

FUNDING AND WORK ENVIRONMENT

The successful candidate will join the group of Nicola Marzari (http://theossrv1.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. This multidisciplinary group is at the forefront of development and applications of materials simulations. It 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), and the work-package on Infrastructure and Interoperability of the H2020 BIG-MAP project (http://www.big-map.eu). Close synergies with the newly created Laboratory for Materials Simulations (LMS, https://www.psi.ch/en/lms) at the Paul Scherrer Institut (PSI) are expected. The group is also actively involved in several international projects, including the H2020 MaX Centre of Excellence (http://www.max-centre.eu), the H2020 projects MarketPlace (https://www.the-marketplace-project.eu), Intersect (http://intersect-project.eu), OpenModel (https://open-model.eu/), DOME 4.0

(https://dome40.eu/), NEP/NFFA (https://www.nffa.eu) together with further national, industrial, and computational projects. Outstanding computing facilities are available both on-site and at CSCS (Switzerland) and CINECA (Italy).

These positions will be funded by the Open Science Platform of MARVEL, dedicated to the promotion of Open Science and of the technologies that enable it, and by the European BATTERY2030+ BIG-MAP project, dedicated to dramatically accelerate battery discovery and innovation.

The contract is initially for 1 year, as required by EPFL, and renewable yearly up to 4 years depending on future funding decisions, and upon mutual satisfaction. Level of employment is 100% on the standard EPFL paygrade (for instance, a gross salary of ~83'000 CHF/year for a recently-graduated PhD).

APPLICATIONS

Candidates should submit two PDF documents: 1) a full CV, including contacts for at least two references and 2) a letter of intent. The documents should be emailed to kristjan.eimre@epfl.ch, giovanni.pizzi@epfl.ch, and nicola.marzari@epfl.ch (a single email simultaneously to all, not three separate emails) with the exact text "BIG-MAP and MARVEL postdoc/software engineer positions" in the subject line. Shortlisted candidates will be contacted individually for initial interviews over Zoom video conferencing. For best consideration, applications should be submitted by March 20th, 2022; the positions will remain open until suitable candidates have been found.