

TWO OPEN POSITIONS FOR COMPUTATIONAL MATERIALS SCIENTISTS/ SOFTWARE SCIENTISTS ON DATA AND SERVICES (THEOS, EPFL)

Two positions for computational materials scientists/software scientists are available at the Ecole Polytechnique Fédérale de Lausanne (EPFL, Lausanne, Switzerland) in the group of Prof. Nicola Marzari. The positions are funded by the new H2020 MarketPlace project (<https://www.the-marketplace-project.eu/>, 2018-2022, 9.2 M€) aimed at developing a single entry point for all industrial and academic materials modelling activities in Europe. EPFL will lead the work package on "Data and Modelling Services".

Outstanding candidates are sought with a background in the physical sciences (typically, physics, chemistry, and materials science) alongside with strong programming abilities and work ethics. Candidates should be comfortable with project management and collaborating with diverse teams around Europe. The project will focus on research case studies for the existing Materials Cloud platform, with primary focus on the portal frontend (in AngularJS) and optimization of its user interface and its ergonomic design, as well as support for the backend development (Python+Flask).

Natural synergies will be present with the AiiDA (<http://aiida.net>) and Materials Cloud (<http://materialscloud.org>) teams, supported by ongoing efforts such as the Swiss National Centre MARVEL (<http://nccr-marvel.ch>) on Computational Design and Discovery of Novel Materials, and the H2020 MaX Centre of Excellence (<http://max-centre.eu>) on Materials Design at the eXascale. In particular, the capability of delivering data-on-demand through AiiDA and containerized or virtualized services through the Materials Cloud are examples of future activities taking place in MarketPlace.

The goal of the MarketPlace project is to leverage recent software engineering and ICT advances to collect, adapt and integrate existing academic and industrial materials modelling components into a single marketplace, to reduce or remove barriers that impede collaboration between academia, SMEs and large enterprises. This entry point will be an interactive online platform which will act as a gateway for a wide range of constituents, enabling them to interact and promote services and expertise.

The first of the two positions will focus on the coordination of the sub projects integrating the various modelling components into the central platform. This role will require strong project management skills, a strong scientific background, but will also demand technical and coding expertise. The second position



will focus more directly on the integration of the diverse components, principally involving the development and utilisation of REST APIs. As such, this role requires a strong technical background ideally with existing knowledge of web frameworks and backend programming (ideally in Python).

Candidates should be interested in working in a field at the intersection between academia and industry, striving to close the gap between the two domains, making state-of-the-art academic modelling tools more easily available for industry, and promoting the European Open Science Platform. For interested applicants, scientific research challenges can also be incorporated where they align with the objectives of the MarketPlace project.

Requirements:

- A PhD in the physical sciences (chemistry, physics or materials). Alternatively, for candidates with an MSc but not holding a PhD degree, a tangible and proven track record in those domains might be accepted as an alternative
- Strong programming skills, not necessarily in any specific language
- The capability to define and implement RESTful application program interfaces
- Strong organisational skills, including the ability to work independently managing complex projects involving multiple partners

Other desirable skills:

- Proficiency in Python
- Experience with cloud services - Amazon AWS, Google Cloud Platform and/or OpenStack
- Web frontend technologies (e.g. AngularJS, React, HTML5, CSS3)
- Modern JavaScript based visualization and UI libraries such as d3.js

The 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. 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 European projects in addition to MarketPlace, including the aforementioned MaX Centre of Excellence (<http://max-centre.eu>), the European Materials Modelling Council (EMMC, <http://emmc.info>) coordination-and-support action, 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.

The group is part of the Quantum ESPRESSO Foundation (<https://foundation.quantum-espresso.org>); in addition to QE, software developed or co-developed in the group includes Wanniergo (<http://wannier.org>), the ENVIRON library for multi-scale electrochemistry (<http://www.quantum-environment.org>), the AiiDA materials' informatics platform (<http://aiida.net>), the GPU library of electronic-structure calculations SIRIUS (<https://github.com/electronic-structure/SIRIUS>) (one open position, soon to be posted), and the Materials Cloud (<http://materialscloud.org>) dissemination platform. Outstanding computing facilities are available on-site and at CSCS (Switzerland) and CINECA (Italy).

Applications:

Candidates should submit 1) a full CV, including contacts for at least two references and 2) a cover letter of intent. These documents (PDF only) should be emailed to giovanni.pizzi@epfl.ch, sebastian.huber@epfl.ch, and nicola.marzari@epfl.ch (all three simultaneously; not three emails) with the exact text "MarketPlace materials scientist" 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 Jul 31st; the positions will remain open until filled. Each position is fully funded for 4 years; the contract is initially for 1 year (as required by EPFL), and renewable for up to 4 years upon mutual satisfaction.

