

OPEN POSTDOC POSITION

INTEGRATION OF THE NANOPOROUS GENOME WITH AiiDA AND THE MATERIALS CLOUD

An open postdoc position is available at EPFL (Sion and Lausanne, Switzerland) in the MARVEL NCCR (<http://marvel-nccr.ch>), a recent Swiss centre for “Computational Design and Discovery of Novel Materials” involving 39 principal investigators (more information is given in the link above). As this is a joint position between the LSMO and THEOS laboratories, the candidate is expected to split his/her time between the two groups.

Excellent candidates are sought with strong experience in the development of software for molecular simulations and an affinity for big-data approaches.

In particular, the project will focus on extending the AiiDA platform (Automated Interactive Infrastructure and Database for Computational Science, www.aida.net) to include the nanoporous materials genome as developed in the LSMO laboratory. AiiDA is a flexible and scalable infrastructure enabling high-throughput simulations, and the main materials’ informatics infrastructure underpinning the efforts of the MARVEL Centre. Moreover, we expect the candidate to contribute to the integration of the research results within the Materials Cloud, a web portal that will be launched soon, dedicated to the sharing of data and workflows, as well as to the dissemination of simulation results managed with AiiDA.

The candidate will work together with a team of physicists, chemical engineers, material scientists and software engineers working either on simulations and applications of nanoporous materials, or developing/contributing to the AiiDA infrastructure and the Materials Cloud portal.

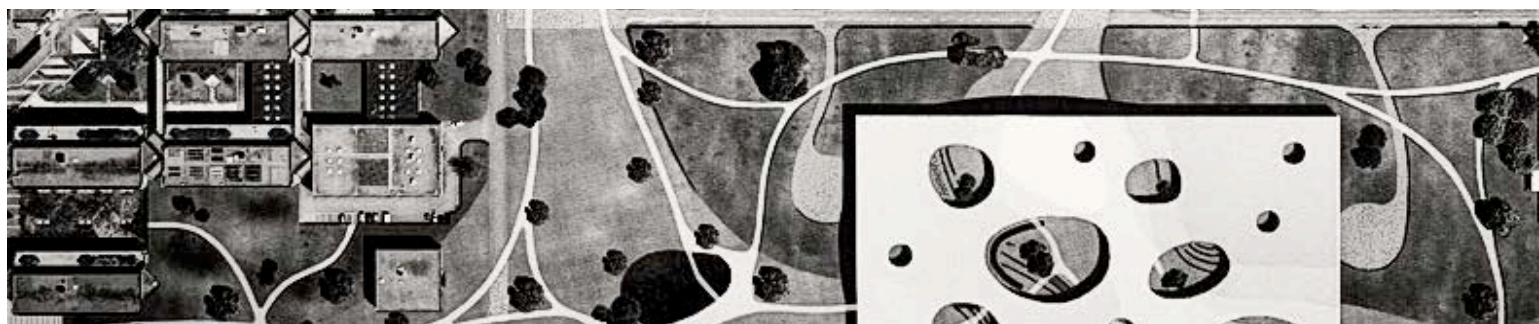
Major duties and responsibilities:

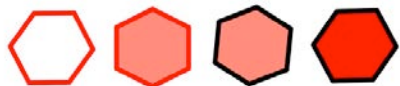
Deliverables of the projects include:

- Integrating of the LSMO libraries of nanoporous materials in the Materials Cloud infrastructure, in particular developing interactive webpages to present curated databases of our nanoporous materials along with their properties
- Develop (web) tools to perform data analysis, like e.g. similarity matching of pore structures
- Develop AiiDA workflows to automate new simulations for the prediction and discovery of new porous materials and of their properties
- Be the link between researchers and AiiDA developers, and provide support to researchers, feedback, and help in development

Skills and experience:

- Experience with molecular simulation techniques (molecular dynamics, Monte Carlo)





- Interest in applications of nanoporous materials (gas separations, gas storage, etc.)
- Experience with at least one between (knowledge of both is an obvious plus):
 - Python: knowledge of basic object-oriented programming concepts (classes, inheritance, ...) and if possible also of a web backend framework, e.g. Flask
 - Web frontend development and technologies (HTML5, CSS3, JavaScript, AngularJS, AJAX, ...)
- Managing codes/projects in a team (version control systems, issue trackers, unit test, continuous integration and other good software practices)

Desirable skills:

- Experience with handling large amounts of data
- Interest in interacting with different groups of researchers

Besides the integration of the nanoporous materials genome effort, the candidate is expected to develop his own research program at the interface of the THEOS and LSMO groups.

Typical candidates will be independent, motivated and enthusiastic, and have a PhD in science or engineering. Moreover, they should be passionate about developing codes and tools both for researchers (to automate simulations and accelerate discovery) and to help present the scientific results to other users in an accessible way.

Preference will be given to candidates with previous experience in similar subjects.

The environment:

The position will be co-hosted in the Laboratory for Molecular Simulations (LSMO), led by Prof Berend Smit (see <http://lsmo.epfl.ch/>) and the Laboratory for Theory and Simulation of Materials, led by Prof Nicola Marzari (see <http://theosrv1.epfl.ch>). EPFL offers a thriving intellectual environment, outstanding computational resources and facilities, and a very lively and active community. THEOS is located in Lausanne, on the shores of Lake Geneva and in close proximity to the Swiss and French Alps, while LSMO in Sion, which is in the middle of the Valais Alps.

Applications:

Candidates should submit a full CV, including contacts for at least two references, and a cover letter of intent to giovanni.pizzi@epfl.ch and berend.smit@epfl.ch, with “MARVEL Postdoc position - nanoporous genome” in the subject line (PDF attachments only). For best consideration applications should be submitted by *January 20th 2017*, but the position will remain open until filled. Shortlisted candidates will be contacted individually for interviews, usually over Skype videoconferencing.

Duration of the contract: 1-year, renewable. Salaries for a postdoc would start typically at ~81,400 CHF.

