

OPEN POSITION: SOFTWARE ENGINEER/DATA SCIENTIST

Integration of AiiDA's Automation Tools and ChemAlive's Cloud Quantum Chemistry Platform

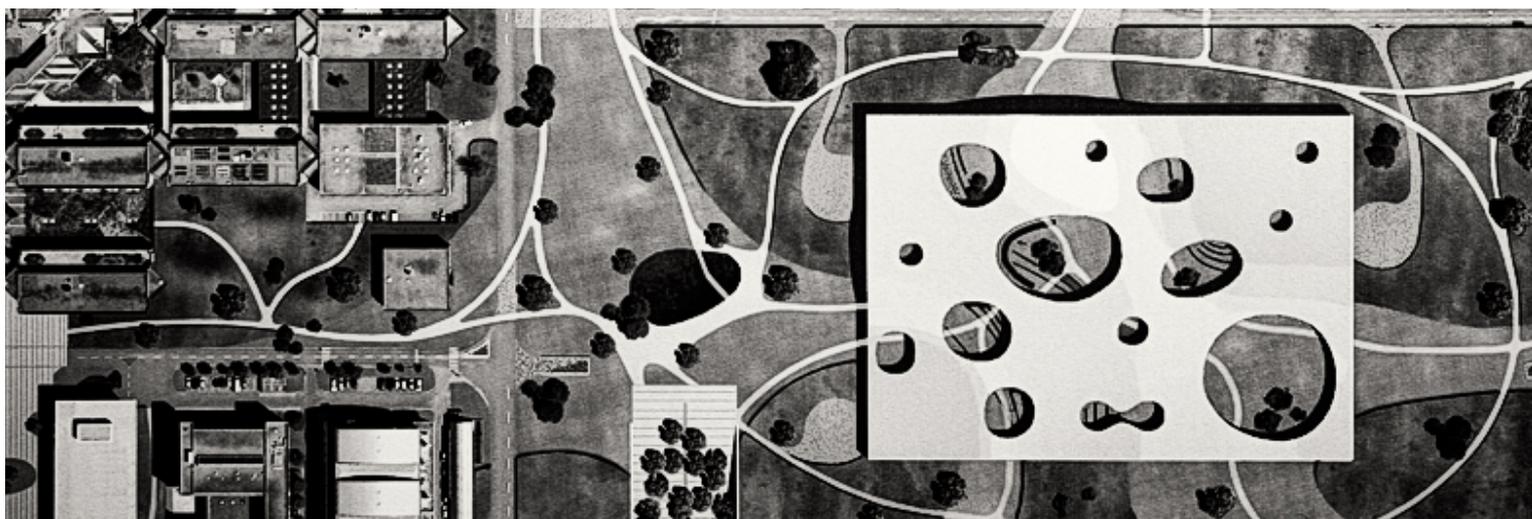
An open position for a software engineer/data scientist is available at EPFL (Lausanne, Switzerland) in the group of Prof. Nicola Marzari and in synergy with the MARVEL NCCR (<http://marvel-nccr.ch>). The position is funded through a partnership with ChemAlive (<http://www.chemalive.com>), a company hosted at EPFL Innovation Park, and the Swiss Commission for Technology and Innovation, through a project grant.

Excellent candidates are sought with strong experience in database architecture and data science, and the development of complex web architectures powered by cloud technologies. A background in physical sciences (chemistry, physics or materials) is a plus with a strong track record in programming.

ChemAlive, as part of its portfolio, develops an on-line web interface for the automation of quantum chemistry codes directly from 2D chemical syntax providing a fully interactive experience in navigating the resulting data in a web environment.

AiiDA (<http://www.aiida.net>) is a materials' informatics framework that acts as a flexible and scalable infrastructure to manage high-throughput computations; Materials Cloud is a portal for computational materials science and an online cloud platform, while ChemAlive is an external commercial partner developing similar technology for molecular chemistry. Such infrastructure underpins the efforts of the MARVEL NCCR; close collaborations also take place with the H2020 Centre of Excellence MaX for "Materials Design at the Exascale" (<http://www.max-centre.eu>).

The primary goal of the current 1.5-year project is to integrate the AiiDA (www.aiida.net) platform into the ChemAlive interface. This will entail coding plugins for common open-source quantum chemistry packages (NWchem, CP2K) and re-coding and further development of workflows developed by ChemAlive into the workflow engine of AiiDA to accomplish complex automation routines using a Python scripting environment.



The position will require direct and frequent communication between the groups working at EPFL, (THEOS/MARVEL and ChemAlive) and Basel (Prof. Anatole von Lilienfeld), and occasional travel between Lausanne and Basel.

The software engineer will work directly with ChemAlive SA employees, and should have a future interest in commercializing computing in chemistry and in on-line science. For interested applicants scientific research challenges can also be incorporated into the effort, but only in so far as they align with the ChemAlive objectives.

Requirements:

- Python experience (advanced)
- Database systems (at least one, ideally PostgreSQL)
- Management of large codes/projects in a team (version control systems, issue trackers, unit test, continuous integration and other good software practices)
- Experience with handling large amounts of data

Other desirable skills:

- Experience with cloud services - Amazon AWS, Google Cloud Platform or OpenStack
- Web frontend technologies (AngularJS, HTML5, CSS3) and web/UI frameworks
- Modern JS visualization and UI libraries (three.js, d3.js, ...)

The software engineer will be based in the Marzari laboratory, and work with a team of 10+ PhD students, postdocs, and software specialists with diverse backgrounds (physicists, chemists, materials scientists and computer scientists) contributing to the AiiDA platform, and would interact closely with the CEO, COO and CTO of ChemAlive (all chemists) as well as the company-side engineers who will be managing the front-end development.

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 both giovanni.pizzi@epfl.ch and p.jarowski@chemalive.com, with the exact text "ChemAlive Database Engineer" in the Subject line.

For best consideration, applications should be submitted by December 10 2017; the position will remain open until filled. Duration of the contract: 1.5 years, with the possibility to renew through future grants and strong possibility of direct hire to ChemAlive, located in Lausanne. Salary strongly competitive compared to standard postdoctoral remuneration.

