

CECAM (<http://www.cecam.org/>) invites applications for a Postdoctoral Researcher position in the area of computational materials science and biosimulations. The Researcher will be based at CECAM HQ in EPF-Lausanne and will work in close collaboration with the developers of the Open Databases Integration for Materials Design (OPTIMADE) consortium (<https://www.optimade.org>). The Postdoctoral Researcher is expected to play a central role in expanding the current capabilities of the OPTIMADE REST API, targeting in particular classical molecular dynamics and bio-simulations.

Some specific objectives are to:

- include the possibility to have a collection of connected structures (e.g. by MD trajectory);
- develop tools to automatically test the existing implementations to verify that they comply to the OPTIMADE specifications;
- develop a systematic approach to deal with metadata and parsing based on well-established community codes.

The appointment will be made for 1 year in the first instance. The gross annual salary for a freshly graduated postdoc is in the range CHF 84 000-90 000, but the salary depends on the successful candidate's level of prior experience. The project allows for extension of at least one year, subject to work assessment and funding decisions.

## Project Outline

Thanks to the exponential growth of computer power and the development of robust codes, it has become possible to perform large sets of calculations automatically. This is the burgeoning area of high-throughput computation. Such calculations have been used to create substantial databases containing the calculated properties of existing and hypothetical materials, many of which have appeared online: the AFLOW distributed materials property repository, the Harvard Clean Energy Project Database, the Materials Cloud, the Materials Project, the NoMaD (Novel Materials Discovery) Repository, the Open Quantum Materials Database, the Computational Materials Repository, the Data Catalyst Genome, ...

The current landscape of data produced in atomic and molecular simulations, however, is quite fragmented and advancement of repositories and analytic tools differs in different areas, e.g. material vs biological modelling. In some of those cases, a Representational State Transfer (REST) Application Program Interface (API) is available to interrogate the database through scripts (though not always documented). So far, however, it is only possible to interrogate one database at a time and the APIs vary from one database to another. Furthermore, the lack of data standards in materials complicates gaining insights from large-scale materials data. Flexible, uniform, computer-readable data standards should be established to enable data to be shared and systematically mined or machine learned.

CECAM has determined to foster and coordinate, in collaboration with state-of-the-art initiatives, the development of open tools of transversal interest in its broad scientific community in the area of data repositories and analysis. In this context, a collaboration has been established with the OPTIMADE consortium to implement a set of specific actions. The OPTIMADE consortium aims to make materials databases interoperational by developing a common REST API. Building on the results already achieved by the consortium, the Postdoctoral Researcher will further develop the OPTIMADE API working specifically on:

- its extension to classical molecular dynamics or biomolecular simulations;
- the development of automatic testing tools of existing OPTIMADE implementations;
- develop a systematic approach to deal with metadata and parsing based on well-established community codes.

After gaining the necessary expertise, the successful candidate will:

- Interact as much as possible with groups across Europe involved in classical molecular dynamics or biomolecular simulations to:
  - present the current OPTIMADE specifications;
  - discuss the recently proposed extension to collections of connected structures;

- gather suggestions for possible changes in the specifications;
- report about the achieved progress at the monthly web meetings of the OPTIMADE consortium and at the group meetings at CECAM HQ;
- participate to the OPTIMADE workshops to present their work and actively contribute to the discussions;
- take initiatives to develop their own career and competences within the project framework;
- contribute to the development of CECAM's activities in the area of Data repositories and analysis.

## Requirements

- A Ph.D. involving research in computational materials science and/or method development.
- Candidates with physics, chemistry, and materials science backgrounds, or equivalent subsequent research experience, are welcome.
- Excellent knowledge of Python (or, at least, of one object-oriented programming language).
- Knowledge of JavaScript and Node.js is welcome and will be taken into account in the selection process but is not required.
- Expertise in the management and the use of databases and in the best practices of API design is considered a plus.
- Excellent spoken and written English.
- Courtesy and respect for all colleagues and collaborators.
- The desire to advance computational materials science at a global level and to take the risk and responsibility of carrying out adventurous and original research.

## How to apply

All communication concerning this opportunity should be sent to **sara.bonella@epfl.ch** and **gianmarco.rignanese@uclouvain.be** with subject line 'Postdoctoral Researcher CECAM-OPTIMADE'. Applications must take the form of one single pdf document, comprising:

- A curriculum vitae / résumé including a complete list of publications and relevant outputs,
- academic degree results and/or rankings, and any awards, distinctions or relevant experience.
- A cover letter explaining your motivation for applying, and your career goals and plans.
- A link to a sample of your own scientific writing, e.g. one paper or research thesis chapter.
- Contact details of two referees who are informed, willing, and available for contact in regard to your application.

The position will remain open until a suitable candidate is identified. Expected start date of employment, March 1 2021.

## Equal Opportunities Policy

CECAM is an equal opportunity employer and is committed to employment policies, procedures and practices which do not discriminate on grounds such as gender, civil status, family status, age, disability, race, religious belief or sexual orientation. We encourage and welcome talented people from all backgrounds to join our staff community.