



EPFL

THEOS
THEORY AND SIMULATION
OF MATERIALS



NCCR
Catalysis

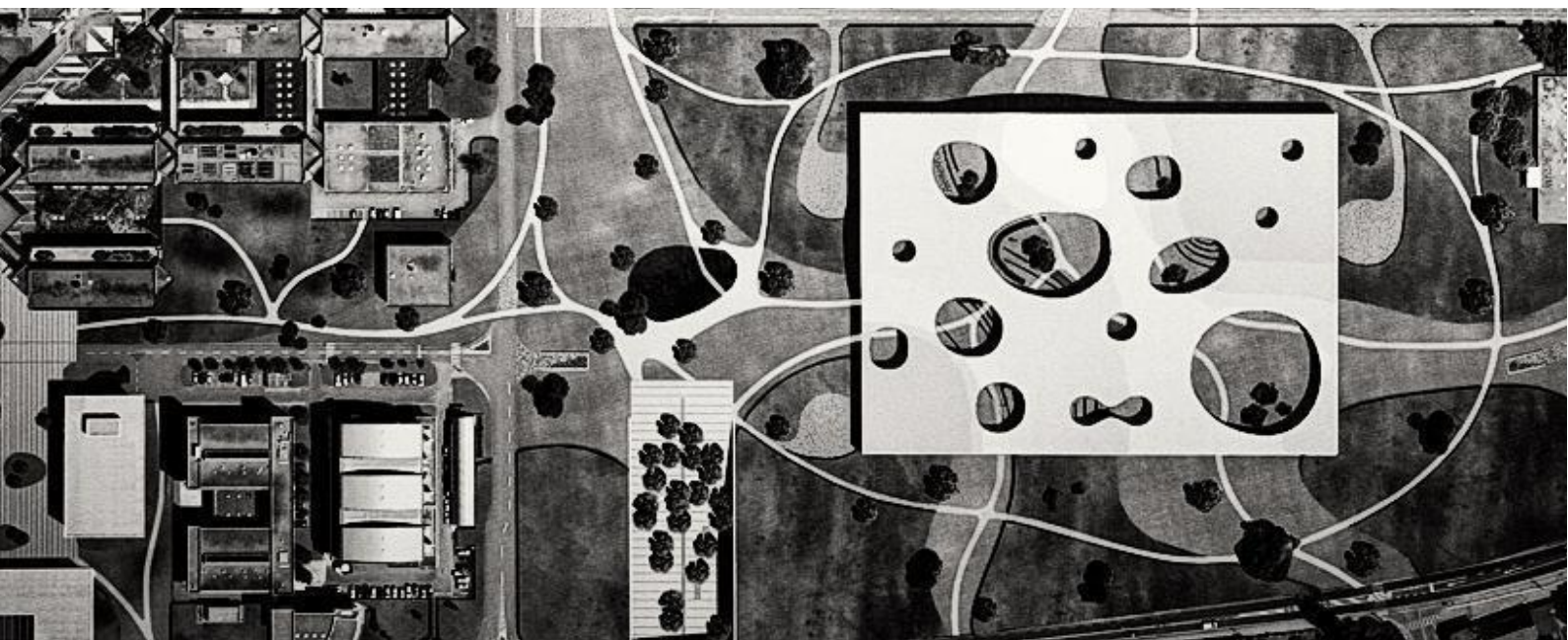
TWO POSTDOCTORAL/PHD POSITIONS ON FIRST-PRINCIPLES OPERANDO SPECTROSCOPIES (THEOS & MARVEL, EPFL)

Two postdoctoral positions are available at the École Polytechnique Fédérale de Lausanne (Lausanne, Switzerland) in the [group of Prof. Nicola Marzari](#). The positions are supported by the new H2020 project [BIG-MAP](#) (Battery Interface Genome – Materials Accelerated Platform, part of the [Battery 2030+](#) initiative), and by the new Swiss National Centre for Competence in Research [NCCR Catalysis](#).

Outstanding and driven candidates are sought with a background in the physical or engineering sciences (physics, chemistry, materials, ...), with passion and commitment to the field, and with a commensurate academic record. Expertise in the development and application of first-principles techniques is required.

The positions are renewable yearly and funded for up to 3 years; they can also be extended to a fourth year upon availability of funding. While typically suited to a postdoctoral appointment, appointments at the PhD level (4 years) would also be appropriate for candidates with a strong, demonstrable track record in the development of electronic-structure simulations.

Natural synergies will be present with the Swiss National Centre [MARVEL](#) on Computational Design and Discovery of Novel Materials and the H2020 [MaX Centre of Excellence](#) on Materials Design at the eXascale; collaborations with the group of [Prof. Oliviero Andreussi](#) at University of North Texas or other electronic-structure research groups in the field are also possible and welcome.





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Objectives: depending on skills and desires, each position could be focused more on the development of novel capabilities, or in the deployment and application of current ones. Broadly, the two positions will contribute to these 3 goals:

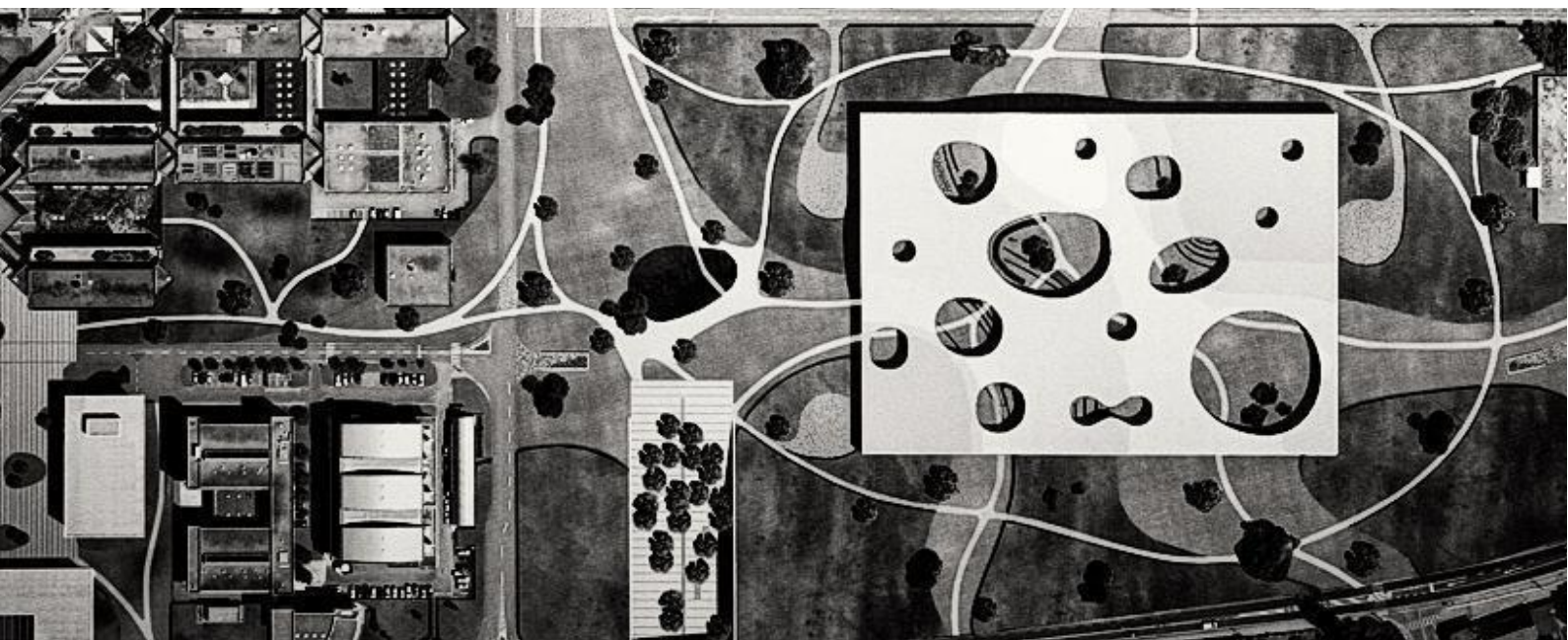
1. **Quantum simulations in electrochemical environments:** development and/or dissemination of electronic-structure simulations using the open-source [Quantum ESPRESSO](#) distribution and the [ENVIRON](#) library for embedding quantum simulations in the appropriate electrochemical environment.
2. **First-principles operando spectroscopies:** development and application of established or novel capabilities for first-principles operando spectroscopies - case studies could be IR/Raman, XAS, ARPES, or NMR.
3. **Open science:** integration of these capabilities into automated solutions that can be deployed locally (e.g. via the use of the [Quantum Mobile](#)) or directly on the web and cloud resources through [AiiDALab](#), for open-access use and dissemination.

Requirements:

- For postdoctoral applicants, a PhD in the physical or engineering sciences (physics, chemistry, materials, ...); for PhD applicants, a MSc in the same fields
- In all cases, a demonstrable and commensurate track record in the development and application of electronic-structure simulations

Other desirable skills:

- Python; experience with AiiDA, AiiDALab, or JupyterLab





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The work environment: The successful candidates will join the group of Nicola Marzari ([Theory and Simulation of Materials](#)) 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. Outstanding computing facilities are available on-site and at [CSCS](#).

Applications: Candidates should submit 1) a full CV (including official or unofficial BA/MSc transcripts), 2) contact information for two to four references and 3) a cover letter of intent. These documents should be emailed to nicola.marzari@epfl.ch with a single PDF attachment, with the exact text "Operando" in the subject line. Shortlisted candidates will be contacted individually for initial interviews, first via video conferencing.

For best consideration, applications should be submitted by **June 15 2021**; the position will remain open until filled. The contract is renewable every year (as required by EPFL) up to a maximum of 4 years, upon mutual satisfaction. Gross postdoctoral salaries for a freshly minted Ph.D. start at 83'600 CHF/year (~76'500 EUR/year), and for a doctoral student at 52'400 CHF/year, with yearly increases of 1500/1000 CHF respectively. Social benefits (unemployment, pension) are also provided.

