



The [Paul Scherrer Institute](#) (PSI) is the largest research institute for natural and engineering sciences in Switzerland. We perform cutting-edge research in the fields of matter and materials, energy and environment, and human health. By performing fundamental and applied research, we work on sustainable solutions for major challenges facing society, science and economy. PSI is committed to the training of future generations. Therefore, about one quarter of our staff are post-docs, post-graduates or apprentices. Altogether, PSI employs 2100 people.

The Paul Scherrer Institute PSI has expanded its focus areas and established a new research division: [Scientific Computing, Theory and Data](#). In recognition of the importance and globally unique ensemble of large facilities at PSI, a key mission for the new division is to support PSI operations and experiments with their increasing challenges and opportunities for a unique digital environment.

Within this division, [a number of laboratories](#) are dedicated to the development and application of the computational and data capabilities that can support and enhance the activities of PSI. The [Laboratory for Materials Simulations](#), directed by Professor Nicola Marzari ([EPFL](#) and PSI), and in close collaboration with the Swiss National Center for Computational Design and Discovery of Novel Materials ([NCCR MARVEL](#)) hosts three groups (“Materials Software and Data”, “Multiscale Simulations”, and “Light-matter Interactions”), whose [mission](#) is to develop, integrate and disseminate in the PSI community and the scientific community at large the computational capabilities required to understand, predict, and characterize materials studied at PSI with photons, neutrons, muons and electrons.

We are currently hiring two tenure-track scientists for the group [Materials Software and Data](#), led by Dr. Giovanni Pizzi. The group will also be complemented by ~6-8 postdoctoral researchers that will join in the forthcoming months. The advertisement below describes one of the two tenure-track openings, focused on the structural, vibrational, electronic, and magnetic properties of complex materials, and their spectroscopies.

Tenure-track Scientist: Electronic-structure simulations of complex materials

SCD Division / Laboratory for Materials Simulations /
Materials Software and Data Group

Your tasks

You will work in an interdisciplinary, multinational research environment and collaborate with your team members and the PSI scientific community. Part of your responsibilities will be

- to develop and sustain a long-term effort in the open-source development of electronic-structure methods able to describe with accuracy the structural, vibrational, electronic, and magnetic properties of complex materials

- to contribute to the development, integration, and dissemination of the computational capabilities required to understand, predict, and characterize materials as studied at PSI with photons, neutrons, muons and electrons
- to provide support and access to these computational capabilities for the PSI science and user programs
- to deliver and curate the computational data for structures, properties and spectra required to discover or design materials with novel or enhanced properties and performance
- to perform your own research at the forefront of computational materials science
- to apply for extramural funding
- to supervise/co-supervise postdoctoral researchers and PhD and M.Sc. students

Your profile

- PhD in physics or a similar domain
- Proven capabilities in the development and dissemination of advanced electronic-structure methods, and in their application to characterize the ground and/or excited states of complex materials
- Record of collaborations in materials' characterization with first-principles calculations
- In-depth postdoctoral experience
- Experience with grant funding/management is desirable
- Experience with supervision of junior researchers (MSc, PhD) is desirable
- Good written and spoken English
- Good written and spoken German or willingness to learn it

We offer

Our institution is based on an interdisciplinary, innovative and dynamic collaboration. You will profit from a systematic training on the job, in addition to personal development possibilities and our pronounced training culture. If you wish to optimally combine work and family life or other personal interests, we are able to support you with our modern employment conditions and the on-site infrastructure. The position is on a tenure-track basis, leading to a permanent position after a successful evaluation after a maximum of 5 years.

Paul Scherrer Institut
 Human Resources Management
 René Gröbli
 Forschungsstrasse 111
 5232 Villigen PSI, Switzerland
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For further information, please contact Prof. Nicola Marzari and/or Dr. Giovanni Pizzi; e-mail: nicola.marzari@psi.ch , giovanni.pizzi@psi.ch

Please submit your application online by 31 January 2023 for this position of Tenure-track Scientist in the Materials Software and Data Group (Index No. 7301-00, <https://www.psi.ch/en/pa/job-opportunities/>), including a CV, application letter, research plans (up to 5 pages), publication list, and contact information for 3 references.



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Tenure-track Scientist: Electronic-structure simulations of excited-state properties

SCD Division / Laboratory for Materials Simulations /
Materials Software and Data Group

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You will work in an interdisciplinary, multinational research environment and collaborate with your team members and the PSI scientific community. Part of your responsibilities will be

- to develop and sustain a long-term effort in the open-source development of electronic-structure methods able to describe with accuracy the electronic, optical, and magnetic excitations of complex materials

- to contribute to the development, integration, and dissemination of the computational capabilities required to understand, predict, and characterize materials as studied at PSI with photons, neutrons, muons and electrons
- to provide support and access to these computational capabilities for the PSI science and user programs
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- to perform your own research at the forefront of computational materials science
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