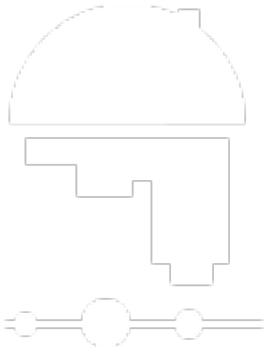
# EUSpecLab/PSI school on advanced spectroscopy



**Monday 15 April 2024 - Friday 19 April 2024**

**Paul Scherrer Institut**

# Scientific Programme

Scope

Spectroscopy is central to the natural sciences and engineering as one of the primary methods for investigating the real world, particularly in characterising the properties of molecules and materials. Varying the energy of the spectroscopic probe gives access to the internal states and dynamics of physical systems. Experimental and theoretical spectroscopy methods go hand in hand to discover new materials and their functions. In addition, machine learning, which is currently revolutionizing the sciences and engineering, has the potential to trigger a paradigm shift, towards algorithm and data driven spectroscopy.

The EUSpecLab spectroscopy school at PSI (the third in a series of EUSpecLab training schools) is geared at PhD students in physics and materials science with basic knowledge in theoretical modelling of modern materials. The school will discuss contemporary research topics in condensed matter and how advanced experimental and theoretical spectroscopic methods are applied to understand complex phenomena and to discover new materials. Topics range from structure determination and ground state properties to advanced concepts like strongly correlated electrons, topology, structural, chemical or dynamic disorder, initial and final state effects and response to static or ultrafast external applied fields.

Topics

Advanced spectroscopy
Angle, spin and time resolved photoelectron spectroscopy (ARPES)
Optical spectroscopy
Pump-probe techniques
Condensed matter physics
Atomic and electronic structure
Spin-orbit interactions, topology
Electron-electron and electron-phonon interactions
Strongly correlated electron systems
Quantum materials
Transition-metal dichalcogenides
Transition metal oxides
Molecules on surfaces
Machine learning methods
Materials discovery
Atomistic simulations
Machine learning potentials
Experiment and Theory
Large research facilities

Confirmed Invited Speakers

Jörg Behler, RU Bochum (DE), Four Generations of Machine Learning Potentials
Michele Ceriotti, EPFL Lausanne (CH), Modeling vibrational and electronic spectroscopies with atomic-scale machine learning
J. Hugo Dil, EPFL Lausanne (CH), Spin-resolved ARPES: from topological materials to quantum interference
Roberto Gunnella, U Camerino (IT), Photoelectron diffraction at low kinetic energy as a high sensitive tool in 2D van der Waals systems
Nicola Marzari, EPFL Lausanne (CH), Materials cloud
Claude Monney, U Fribourg (CH), Time-resolved ARPES: Observing photoinduced phase transitions and excited states
Daniele Passerone, Empa Dübendorf (CH), Computational science in a materials and nano-science laboratory
Nicholas C. Plumb, PSI (CH), Viewing quasiparticle behavior through the ARPES spectral function
Milan Radovic, PSI (CH), Spectroscopy images exotic electronic systems and experiences interplay between different emerging phenomena in Transition Metal Oxides
Nicolas Schmid, ZHAW Winterthur (CH), Machine learning in NMR spectroscopy
Michael Schüler, U Fribourg (CH), Time-resolved ARPES
Ari P. Seitsonen, CNRS Paris (F), Molecules on surfaces

Vladimir N. Strokov, PSI (CH), Advanced topics in ARPES: Final-state effects and high-energy photoemission
Alea M. Tokita, RU Bochum (DE), How to train a neural network potential
Chiara Trovatello, Columbia U (US), Exploring the nonlinear optical response of 2D semiconductors
Tian Xie, Microsoft Research (UK), MatterGen: a generative model for inorganic materials design
Contributions

All participants are invited to present a poster. Some of the contributions may be selected for an oral presentation.