Sunstar Hotel Grindelwald
Dorfstrasse 168
3818 Grindelwald

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Distances

Centre	300 m
Train station	500 m
(contact the hotel in advance if you need a hotel bus pickup)	
Bus station (“Firstbahn”)	vis-à-vis
Firstbahn gondola	vis-à-vis

MARVEL Review and Retreat 2026

Program

January 12-14, 2026

Sunstar Hotel, Grindelwald

MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

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Swiss National Science Foundation

The National Centres of Competence in Research (NCCR) are a funding scheme of the Swiss National Science Foundation

Monday, January 12, 2026

Free arrival – Official check-in time 16:00 (usually possible earlier if room available)

16:15 **Welcome and introduction**
Nicola Marzari (MARVEL Director, EPFL/PSI)

16:35 **Pillar 1 | Design and discovery of novel materials**
- Anirudh Raju Natarajan (EPFL): *Pillar 1 overview*
- Pandula Manura Liyanage (EPFL): *Design of multi-component BCC refractory alloys with high strength and high ductility: Theory and simulation*
- Julia Chmielewska (Empa): *Alloy Design and Mechanical Behaviour of High-Strength–Ductility Hf–Mo–Nb–Ti Refractory HEA*
- Vladyslav Turlo (Empa): *OptiMat.Chat: Agentic AI approach to materials research*

17:55 **Pillar 2 | Machine learning platform for molecules and materials**
- Michele Ceriotti (EPFL): *Pillar 2 overview*
- Sofiia Chorna (EPFL): *MAD and the feature space analysis*
- Yannick Calvino Alonso + Romain Graux (EPFL): *LCMD-DB and its connections to the LCMD ecosystem*
- Filippo Bigi (EPFL): *FlashMD: long-stride, universal prediction of molecular dynamics*

19:15 **Dinner**

20:30 **Pub quiz**

Tuesday, January 13, 2026

08:00 **Breakfast**

09:00 **Pillar 3 | Digital infrastructure of open simulations and data**
- Giovanni Pizzi (PSI): *Pillar 3 overview*
- Michail Minotakis (PSI): *Robust high-throughput simulations and materials discovery enabled by MC3D*
- Federica Troni (EPFL): *Mass-Zero constrained molecular dynamics for electrostatic interactions*
- Niklas Schmitz (EPFL): *Algorithmic Differentiation for plane-wave DFT*

10:20 **Coffee break**

10:50 **Industrial careers and technology transfer with the MARVEL Industrial Advisory Board**

11:40 **MARVEL legacy panel**

12:10 **Lunch**

14:00 **Poster session**

16:00 **Coffee break**

16:30 **Pillar 4 | Long-term integration in the Swiss scientific landscape**
- Nicola Marzari (EPFL/PSI): *Pillar 4 overview*
- Aliaksandr Yakutovich (Empa): *AiiDAlab: on the route to accelerate science*
- Alberto Carta (PSI): *Hunting down the ground state: balancing exploration and exploitation in magnetic landscapes*
- Nicola Colonna (PSI): *Koopmans spectral functionals for band structure, electron–phonon coupling, and real-time electronic dynamics*

17:50 **End of talks**

19:00 **Dinner**

20:30 **Socializing, drinks & board games (hotel lobby)**

Wednesday, January 14, 2026

08:00 **Breakfast**

09:00 **Advanced simulation methods**

- Philipp Werner (Uni Fribourg): *Project overview*
- Gian Parusa (PSI): *Angle-resolved photoemission spectroscopy from first principles*
- Manasa Kaniselvan (ETHZ): *Bridging computational materials science and semiconductor device simulations by learning electronic material properties at scale*
- Ruslan Mushkaev (Uni Fribourg): *Strange metallicity in a Kagome metal, a DMFT perspective*

10:20 **Coffee break**

10:50 **Leveraging quantum computers and algorithms for materials discovery**

- Giuseppe Carleo (EPFL): *Project overview*
- Samuele Piccinelli (IBM): *Quantum chemistry with provable convergence via randomized sample-based quantum diagonalization*
- Gian Gentinetta (EPFL): *Quantum Finite Temperature Lanczos Method*
- Julia Gerecke (EPFL): *Ground-State Preparation for Spin and Fermionic Systems using Operator Propagation Methods*

12:10 **Q&A with the MARVEL Scientific Advisory Board**

12:40 **Lunch**

14:00 **Private session (Scientific/Industrial Advisory Boards + Executive Committee only)**
Discussion and feedback

List of posters

Pillar 1 | Design and discovery of novel materials

1 *First-principles models of defects in alloys* — Deepak Somani (EPFL)

2 *First-Principle Thermodynamics of Multicomponent Alloys* — Yann Müller (EPFL)

3 *First-principles thermodynamics of hydrogen absorption in binary C15 Laves phases* — Claire Paetsch (EPFL)

Computational design and discovery of novel materials (going beyond the theme of pillar 1)

4 *Data-driven flammability predictions for organics*— Jiaqi Zhou (EPFL)

5 *Voltage Profile Predictions for Na-Ion Cathodes: A Hybrid MLIP–PBEsol+U+V approach* — Stefan Schären (PSI)

6 *Score-based diffusion models for accurate crystal structure inpainting and reconstruction of hydrogen positions* — Timo Reents (PSI)

7 *High-throughput simulations of Fermi surfaces and quantum oscillation frequencies from first principles* — Nataliya Paulish (PSI)

8 *Charting the landscape of Bardeen-Cooper-Schrieffer superconductors in experimentally known compounds* — Marnik Bercx (PSI)

9 *Charting the electronic structure of experimentally known inorganic crystals* — Junfeng Qiao (EPFL), Maria Andolfatto (PSI), Szymon Blazucki (PSI)

Pillar 2 | Machine learning platform for molecules and materials

10 *Unconstrained models for electronic structure* — Pol Febrer Calabozo (EPFL)

11 *FlashMD: long-stride, universal prediction of molecular dynamics* — Filippo Bigi (EPFL)

12 *Lightweight, universal machine-learning models for atomistic materials simulations* — Arslan Mazitov (EPFL), Cesare Malosso (EPFL)

13 *Long-range models* — Philip Loche (EPFL)

List of posters *(cont.)*

Pillar 2 *(cont.)*

14 *Physics-Inspired Machine Learning Models for Transition Metal Complexes with Diverse Charge and Spin States* — Yuri Cho (EPFL)

15 *Pillar 2: machine learning platform for materials discovery* — Liam Marsh (EPFL)

16 *Structural Characterization of Amorphous Drug Formulations* — Jacob Holmes (EPFL)

Pillar 3 | Digital infrastructure of open simulations and data

17 *Enhancing AiiDA's user experience: recent developments and improvement* — Edan Bainglass (PSI), Xing Wang (PSI)

18 *Multi-fidelity and -objective optimization of ONCV pseudopotentials* — Austin Zadoks (PSI)

19 *Materials Cloud: recent updates and plans for long-term sustainability* — Bud Macaulay (PSI)

20 *Lhumos: Learning Hub for Modelling and Simulation*— Roberto Bendinelli (EPFL)

21 *Discretization Error Quantification in Plane-Wave Density Functional Theory* — Bruno Ploumhans (EPFL)

22 *Milestones in Software Development for an Open Digital Infrastructure* — Simon Pintarelli (CSCS)

Pillar 4 | Long-term integration in the Swiss scientific landscape

23 *Understanding the anionic redox activity in layered Na-ion battery cathode materials* — Valentina Sanella (PSI)

24 *Leveraging Wannierization and linear-response Hubbard parameterization to derive many-body models for carbon-based nanostructures* — Gonçalo Catarina (Empa)

25 *Examples of AiiDAlab Quantum ESPRESSO app usage in the nanotech@surfaces laboratory of Empa* — Andres Ortega-Guerrero (Empa)

26 *xc-functional dependence of the local screened Coulomb interaction and the dynamical Hubbard functional* — Mario Caserta (EPFL)

27 *Quantum annealing for materials science* — Alfredo Fiorentino (PSI)

28 *AiiDAlab@PSI: A Unified Platform for Simulations and Experimental Data Analysis* — Miki Bonacci (PSI)

Advanced simulation methods

29 *Pump-induced out-of-equilibrium magnetism in the Mott insulator CuO* — Katja Sophia Moos (PSI)

30 *Optimal Local Orbitals: A systematic approach for Accurate Wave Function Representation* — Ann Chantal Goutier (PSI)

31 *First-principles modeling of electron tunneling in van der Waals heterostructures* — Nicolas Vetsch (ETHZ)

32 *Strongly correlated physics in organic open-shell quantum systems* — Anooja Jayaraj (Empa)

Leveraging quantum computers and algorithms for materials discovery

33 *Predicting Topological Entanglement Entropy in a Rydberg analog simulator* — Linda Mauron (EPFL)

34 *Algorithms for quantum spin systems* — Yanting Teng (EPFL)

35 *Precise Quantum Chemistry calculations with few Slater Determinants* — Clemens Giuliani (EPFL)