

PROGRAM

**Department of Materials Science
Montanuniversität Leoben**

**5th Materials Science Colloquium
70. Metallkunde-Kolloquium
Lech am Arlberg
13. – 17. April 2026**

Highlight Topic:
Artificial Intelligence (AI) in Materials Science

**Welcome Reception with Pfefferkorn Family:
Monday, April 13th, 2026, 18.30 h**

Organization:

Department of Materials Science
Montanuniversität Leoben
A-8700 Leoben, Roseggerstraße 12

Steering Committee:

Prof. Raul Bermejo
Prof. Jürgen Eckert
Prof. Daniel Kiener
Prof. Christian Mitterer
Prof. Lorenz Romaner
Prof. Ronald Schnitzer

Organization Committee:

Dr. Andrea Bachmaier
Priv.-Doz. Dr. David Holec

Program

All presentations will be held in the seminar room of Hotel Krone in Lech am Arlberg.

All presentation times include discussion time,
invited presentations (IP) 25 + 5 min and regular presentations (P) 15 + 5 min.
Due to the full program please keep in time.

Tuesday, 14. April 2026

13.55 Welcome

Chair: Prof. Ronald Schnitzer

14.00 **Trost, C. O. W. (IP)** Rethinking nanoindentation toward explainable machine learning and open science: In situ tip radius estimation and advanced property mapping

Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Austria

14.30 **Zeller-Plumhoff, B. (P)** Utilizing deep learning to study and predict the behaviour of biodegradable magnesium- and zinc-based implants

Data-driven Analysis and Design of Materials, Faculty of Mechanical Engineering and Marine Technologies, University of Rostock, Germany

14.50 **Mayrhofer, P. H. (P)** Data- and physics-driven design of defect-tolerant TiN/MoN and TiN/TaN superlattice coatings

Institute of Materials Science and Technology, TU Wien, Austria

15.10 **Reiners-Sakic, A. (P)** DFT and MLIP study of solute segregation to coherent and semi-coherent α -Fe/Fe₃C interfaces

Christian Doppler Laboratory for Knowledge-based Design of Advanced Steels, Department Materials Science, Montanuniversität Leoben, Austria

15.30 **Greiner, C. (IP)** How to predict friction: A tale of surface topography and machine learning

Institute for Applied Materials (IAM), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

16.00 Group photo & break

Chair: Prof. Daniel Kiener

16.30 **Neugebauer, J. (IP)** Artificial intelligence and data-driven design of materials

Department Computational Materials Design, Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

17.00 **Antretter, T. (P)** Modeling the segregation of intermetallic phases in Pb-free microelectronic solders

Department Physics, Mechanics and Electrical Engineering, Montanuniversität Leoben, Leoben, Austria

17.20 **Gottlieb, H. (P)** Experimental investigation and simulation validation of friction stir welding of thick aluminium 6082-T651

Institute of Materials Science, Joining and Forming, TU Graz, Austria

17.40 **Gupta, V. (P)** Workflow for automated information extraction from materials science literature using ontology-guided reflective AI agents: A γ -TiAl creep case study

Helmholtz Zentrum Hereon, Geesthacht, Germany

18.00 **Belferkous, B. A. (P)** From spectra to insight: Multivariate analysis of NIR data for early degradation detection in photovoltaic materials

Polymer Competence Center Leoben GmbH (PCCL), Leoben, Austria

18.20 **Staudacher, M. (P)** Bayesian optimization of laser-aided fracture toughness specimen preparation

Department Materials Science, Montanuniversität Leoben, Austria

18.40 **Ruetz, M. (P)** On the thermo-acoustoelastic effect of Rayleigh waves and its metal physical interpretation

Department Physics, Mechanics and Electrical Engineering,
Montanuniversität Leoben, Austria

19.00 End of presentations

Wednesday, 15. April 2026

Chair: Dr. Claus Trost

14.00	Gumbsch, P. (IP)	Digitalization of materials, the basis for machine learning applications and advanced materials technologies
	KIT, Institute for Applied Materials, Karlsruhe and Fraunhofer IWM, Freiburg, Germany	
14.30	Bucher, E. (P)	AI assisted image analysis as a powerful tool to accelerate materials development for solid oxide electrolyzer cells
	Department General, Analytical and Physical Chemistry, Montanuniversität Leoben, Austria	
14.50	Hu, Y. (P)	AI-driven multiscale modeling of thermal transport in LiCoO ₂ cathode materials
	Laboratory for Advanced Materials Processing, Empa – Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland	
15.10	Pferschy, M. (P)	Under pressure – AI usage for faster simulations of Li-Ion cells
	Department of Polymer Engineering and Science, Montanuniversität Leoben, Austria	
15.30	Schrefl, T. (IP)	AI-accelerated multiscale design of permanent magnets
	Christian Doppler laboratory for magnet design through physics informed machine learning, University for Continuing Education Krems, Wiener Neustadt, Austria	
16.00	Break	

Chair: Priv.-Doz. David Holec

16.30	Mrovec, M. (IP)	Foundational GRACE: Towards quantum accuracy in atomistic modeling of materials
		Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany
17.00	Reichmann, A. (P)	Machine learning model for predicting grain boundary enrichment in ferrite
		Department Materials Science, Montanuniversität Leoben, Austria
17.20	Legenstein, L. (P)	Machine-learned potentials as efficient surrogates for first-principles modeling of organic semiconductors
		Department Physics, Mechanics and Electrical Engineering, Montanuniversität Leoben, Austria
17.40	Turlo, V. (P)	Moving from algorithmic to agentic computing in materials research
		Laboratory for Computational Engineering, Empa, Duebendorf, Switzerland
18.00	Aydin, R. (P)	Large language models in materials science
		Helmholtz-Zentrum Hereon, Geesthacht, Germany
18.20	Scheiber, D. (IP)	Accelerated pathways to discover and apply novel sustainable materials solutions with AI
		Materials Center Leoben Forschung GmbH, Leoben, Austria
18.50	End of presentations	

Thursday, 16. April 2026

Chair: Prof. Dr. Clara Schuecker

14.00	Messiha, M. (IP)	Bypassing trial-and-error: From 1000 hours to rapid prediction of recycled PP blends
	PolyDecypher FlexCo, Leoben, Austria	
14.30	Danninger, L. R. (P)	Bayesian optimization applied to the parameterization of Crystal Plasticity models
	Laboratory of Simulation and Multiscale Materials Modelling, Federal University of ABC, Santo André, Brazil	
14.50	Pettermann, H. E. (P)	Constitutive modeling of anisotropic elasto-damage materials – a data driven machine learning approach
	Institute of Lightweight Design and Structural Biomechanics, TU Wien, Austria	
15.10	Kostwein, N. (P)	Linking grain boundary segregation to embrittlement: Experimental and first-principles analysis of tramp elements in 51CrV4 steel
	Christian Doppler Laboratory for Knowledge-based Design of Advanced Steels, Department Materials Science, Montanuniversität Leoben, Austria	
15.30	Schwarz-Gsaxner, A. (IP)	From process to product: Structured flow data as a foundation for AI applications
	voestalpine Forschungsservicegesellschaft Donawitz GmbH. Leoben	
16.00	Break	

Chair: Dr. Andrea Bachmaier

16.30	Ramadan, Z. (IP)	Multiphysics simulations and machine learning of thermal fields and mass transport in SiC crystal growth in PVT furnaces
	Christian Doppler Laboratory of Advanced Computational Design of Crystal Growth, Department Materials Science, Montanuniversität Leoben, Austria	
17.00	Hatzenbichler, L. (P)	Effects of tramp elements in recycled steels supported by AI-assisted microstructural analysis
	Christian Doppler Laboratory for Knowledge-based Design of Advanced Steels, Department Materials Science, Montanuniversität Leoben, Austria	
17.20	Müller, M. (P)	Advancing AI-driven microstructure analysis through correlative microscopy approaches
	Department of Materials Science and Engineering, Saarland University, Saarbrücken, Germany	
17.40	Keckes, J. F. (P)	Beyond load-displacement: Leveraging computer vision for in situ micromechanical testing experiments
	Department Materials Science, Montanuniversität Leoben, Austria	
18.00	Wechner, N. (P)	Hybrid segmentation model for detecting Fe-rich intermetallic phases in secondary aluminium alloys
	Department Metallurgy, Montanuniversität Leoben, Austria	
18.20	Munz, M. (P)	Automated microstructure analysis through image segmentation using a neural network
	Department Materials Science, Montanuniversität Leoben, Austria	
18.40	Final remarks & announcement of 6th Materials Science Colloquium 2027	

The abstracts and the list of the participants you can find here: