



IC-MPPE 2024

<https://www.ic-mppe2024.org>

Integrated Computational Materials, Process and Product Engineering

IC-MPPE 2024 6.& 7. June 2024 in Leoben, Austria



The conference has been organised in sessions on the following core topics of the IC-MPPE programme:

- **IC-MPPE for Sustainable and Circular Economy for metallic materials**
 - Accelerated materials design
 - Digital and green production
 - Digitalization and reliability of railway vehicles and tracks
 - Condition monitoring and condition-based maintenance
 - High-end material characterization methods;
- **IC-MPPE for energy transport, storage and conversion**
 - Hydrogen transport and storage;
 - Electrical energy storage and conversion;
- **Advanced materials and systems for smart electronics**
 - Reliability of electronic-based systems
 - Sensor development

Conference schedule Thursday, 6.6.2024

start	Congress Hall	
07:30	On-site registration (office in front of the rooms)	
08:30	Opening ceremony & introduction to the IC-MPPE programme	
	Erzherzog Johann Hall	Peter Tunner Hall
09:00	Accelerated materials design I (Chair: Daniel Scheiber)	Hydrogen transport and storage I (Chair: Vsevolod Razumovskiy)
10:20	Coffee break	Coffee break
10:50	Digital and green production I (Chair: Peter Raninger)	Hydrogen transport and storage II (Chair: Vsevolod Razumovskiy)
12:10	Lunch at the conference venue	Lunch at the conference venue
13:30	Accelerated materials design II (Chair: Daniel Scheiber)	Condition monitoring and condition-based maintenance I (Chair: Hans-Peter Ganser)
14:50	Coffee break	Coffee break
15:20	Digital and green production II (Chair: Peter Raninger)	Sensor development (Chair: Anton Köck)
17:00	break	break
	Congress Hall	
18:00	Get-together & Poster Session	
19:00	Conference Dinner	

Thursday, 6.6.2024 - Erzherzog Johann Hall

start	end	Accelerated materials design I		
09:00	09:20	Accelerating the design of sustainable and high performing metallic materials and solutions	Anssi Laukkanen	VTT Technical Research Centre of Finland
09:20	09:40	Radically new possibilities for materials discovery on the materials acceleration platform ALPmat	Jürgen Spitaler	Materials Center Leoben Forschung GmbH
09:40	10:00	Accelerated design of bainitic steels – optimized experimental workflow	Dominik Brandl	Materials Center Leoben Forschung GmbH
10:00	10:20	From Virtual Materials Design to Materials Acceleration Platforms	Wolfgang Wenzel	Karlsruhe Institute of Technology - Institute of Nanotechnology
10:20	10:50	Coffee break		
start	end	Digital and green production I		
10:50	11:10	Trends and needs in the European steel industry for digitalization and decarbonization	Klaus Peters	European Steel Technology Platform (ESTEP)
11:10	11:30	Green steel production and its implications for digitalization	Markus Sonnleitner	voestalpine Stahl GmbH
11:30	11:50	From BOF to EAF: Considering new elements and concentrations for phase transformation kinetics	Bernhard Bloder	Materials Center Leoben Forschung GmbH
11:50	12:10	Development and application of modern prediction models for heavy plate production	Thomas Kaltenbrunner	voestalpine Grobblech GmbH

Personal notes...

Thursday, 6.6.2024 - Peter Tunner Hall

start	end	Hydrogen transport and storage I		
09:00	09:20	Characterizing the fracture micromechanisms of pipeline steels in the presence of hydrogen	Tom Depover	Ghent University - Department of Materials, Textiles and Chemical Engineering
09:20	09:40	Digital material design for hydrogen transport and storage applications	Vsevolod Razumovskiy	Materials Center Leoben Forschung GmbH
09:40	10:00	Industrial challenges related to HISC in Ni-base alloys and austenitic steels	Jan Platl	voestalpine Böhler Edelstahl GmbH & Co KG
10:00	10:20	Hydrogen in (used) pipelines - H ₂ quality, flow dynamics and consequences for the refurbishment	Thomas Stöhr	Hydrogen Research Center Austria (HyCentA)
10:20	10:50	Coffee break		
start	end	Hydrogen transport and storage II		
10:50	11:10	How to design new hydrogen embrittlement resistant materials via atom probe tomography and in-situ nanoindentation	Anna Sophie Jelinek	Montanuniversität Leoben - Department Materials Science
11:10	11:30	Fundamental insights into the mechanism of hydrogen embrittlement	Tilman Hickel	Bundesanstalt für Materialforschung und -prüfung (BAM)
11:30	11:50	Hydrogen transportation and storage: materials issues	Jader Furtado	Air Liquide - Materials Science Group
11:50	12:10	Hydrogen embrittlement of two carbon steels in a 1000 bar hydrogen environment	Gregor Mori	Montanuniversität Leoben - Chair of General and Analytical Chemistry

Thursday, 6.6.2024 - Erzherzog Johann Hall

start	end	Accelerated materials design II		
13:30	13:50	How Machine Learning Interatomic Potentials can advance computer aided materials design	Max Ludwig Hodapp	Materials Center Leoben Forschung GmbH
13:50	14:10	Process and material design of high-performance ODS components for energy transition applications	Michael Mayer	Materials Center Leoben Forschung GmbH
14:10	14:30	Software and data infrastructure for material data management	Heimo Gursch	Know-Center GmbH
14:30	14:50	(canceled)		
14:50	15:20	Coffee break		
start	end	Digital and green production II		
15:20	15:40	Digital design of free forming processes for aerospace components	Aleksandar Stanojevic	voestalpine BÖHLER Aerospace GmbH & Co KG
15:40	16:00	Digitalization of a research "production" lab: Opportunities for upscaling and knowledge transfer	Martin Stockinger	Montanuniversität Leoben - Chair of Metal Forming
16:00	16:20	Current challenges for the automotive sector – Suppliers in a sandwich position between OEM and material producer	Thomas Otten	Robert Bosch GmbH - Engineering Heat Treatment, Metal Technology
16:20	16:40	Optimization of magnetic properties of electrical steel strip along the process chain	Masoud Sistaninia	Materials Center Leoben Forschung GmbH
16:40	17:00	Concepts for offline and inline measurement of material properties based on magnetic excitation	Mohammad Zhian Asadzadeh	Materials Center Leoben Forschung GmbH

Thursday, 6.6.2024 - Peter Tunner Hall

start	end	Condition monitoring and condition-based maintenance I		
13:30	13:50	Demand-oriented street lighting	Gerold Meininger	MEDS
13:50	14:10	Energy-aware condition monitoring of turbine blades on wireless sensor nodes	Manfred Mücke, Lukas Hanna	Materials Center Leoben Forschung GmbH
14:10	14:30	Model order reduction in continuous galvanizing baths	Werner Eßl	Materials Center Leoben Forschung GmbH
14:30	14:50	Hybrid modeling - exploring the field between white-box and black-box modeling	Hans-Peter Ganser	Materials Center Leoben Forschung GmbH
14:50	15:20	Coffee break		
start	end	Sensor development		
15:20	15:40	Spark ablation and impaction printing as a building block for nanostructured-based multifunctional devices: from energy storage and conversion devices up to sensing applications	Leandro Sacco	VSParticle B.V.
15:40	16:00	Chemical Sensors – where to go? Emerging Applications for Environment and Health	Anton Köck	Materials Center Leoben Forschung GmbH
16:00	16:20	Lab-on-Foil Microfluidic Chips for point of care Diagnostics of Corona antibodies fabricated by roll-to-roll UV NIL	Anja Haase	Joanneum Research - Materials - Hybrid Electronics and Patterning
16:20	16:40	Inkjet Printing for Printed Electronics	Peter Bauer	PROFACTOR GmbH
16:40	17:00	Textile-integrated sensor technology and simulation of environmental conditions for testing electronics	Rudolf Heer	Silicon Austria Labs - Sensor Systems

Poster session (Congress Hall)

Poster Title	Name	Surname	Affiliation
MCL - Software as a service	Bedoya-Martinez	Natalya	Materials Center Leoben Forschung GmbH
Micromechanical investigation of lead-free soft solder with in-situ microcompression experiments and advanced nanoindentation	Buchebner	Nadine	Montanuniversität Leoben
Multi-Gas sensor array based on SnO ₂ and CuO thin films functionalized with Ag and Cu nanoparticles	Egger	Larissa	Materials Center Leoben Forschung GmbH
Modeling the Influence of Bainite Transformation on the Mechanical Behavior of Steel	Faraji	Towhid	TU Freiberg
Fully Automated Multiple ML Algorithm Power Measurement and Ranking	Gratl	Christoph	Materials Center Leoben Forschung GmbH
Automatic ARM Code Generation from ML Algorithms Expressed in ONNX	Gratl	Christoph	Materials Center Leoben Forschung GmbH
Laser-Ultrasound for In-Situ Monitoring of Microstructural Changes in Steel	Grünsteidl	Clemens	RECENDT
AI-accelerated materials informatics method for the discovery of ductile alloys	Hodapp	Max	Materials Center Leoben Forschung GmbH
Notes on Digitalisation of Greener Material Processes: Ontology and Data Models	Horr	Amir	AIT
Fatigue crack growth in nanocrystalline nickel micro specimens – crack initiation and short crack growth under geometrical constraint	Jelinek	Alexander	Montanuniversität Leoben
Mapping deformation structures of an AA6061 aluminum alloy with double cone compression tests	Kahlenberg	Robert	Materials Center Leoben Forschung GmbH
Novel chemical sensor device enabled by simultaneous thermal-optical excitation	Köck	Anton	Materials Center Leoben Forschung GmbH
Gas Sensing Performance of CuO Sensors Functionalized with Different Stabilized Au-NP	Maier	Christian	Materials Center Leoben Forschung GmbH
Using Explainable AI in Mechanical Property Prediction Modeling	Millner	Gerfried	Materials Center Leoben Forschung GmbH
KIRAMET - AI-based Recycling of Metal Composite Waste	Neubauer	Melanie	Montanuniversität Leoben
BiMg ₂ /3Nb ₁ /3O ₃ -based thin films from Chemical Solution Deposition – A study on the influence of the process parameters on the structure and electrical properties	Panzic	Ivana	Materials Center Leoben Forschung GmbH
How stress relaxation tests can help to find kinetic parameters for creep simulations	Riedlsperger	Florian	Institute for Engineering Materials
Simulation workflow for digital aluminium sheet production	Shah	Vitesh	AMAG Rolling GmbH
Challenges and Advances in the characterization of LiVPO ₄ : From HR-STEM & EELS to Novel Scanning Diffraction Techniques	Šimić	Nikola	FELMI-ZFE
Artificial intelligence to improve defect detection capabilities of ultrasonic microscopy	Sukumaran Nair	Arya	PVA TePla Analytical Systems GmbH
Measuring the Propagation of Fatigue Cracks Emanating from Microstructurally Small Notches	Walch	Lukas	Materials Center Leoben Forschung GmbH
Alternative PoF-based accelerated testing methods	Walter	Thomas	TU Wien
Pushing the limits of SAM with ML approaches	Wilhelmer	Alexander	Materials Center Leoben Forschung GmbH
Recent progress in the physically-based dislocation creep modelling of P92 covering different temperature and stress ranges	Witzmann	Laura	JKU Linz

Conference schedule Friday, 7.6.2024

start	Erzherzog Johann Hall	Peter Tunner Hall
08:30	Digitalization and reliability of railway vehicles and tracks I (Chair: Jürgen Maierhofer)	Electrical energy storage and conversion I (Chair: Roland Brunner)
09:50	Coffee break	Coffee break
10:20	Digitalization and reliability of railway vehicles and tracks II (Chair: Jürgen Maierhofer)	Electrical energy storage and conversion II (Chair: Roland Brunner)
11:40	Lunch at the conference venue	Lunch at the conference venue
13:00	High-end material characterization methods (Chair: Dominik Brandl)	Reliability of electronic-based systems (Chair: Elke Kraker)
14:20	Coffee break	Coffee break
14:50	Condition monitoring and condition-based maintenance II (Chair: Hans-Peter Gänser)	Reliability of electronic-based systems (Chair: Elke Kraker)
15:50	Closing & final Coffee	Closing & final Coffee

Friday, 7.6.2024 - Erzherzog Johann Hall

start	end	Digitalization and reliability of railway vehicles and tracks I		
08:30	08:50	Novel sensor concepts for railway track condition monitoring	Sven Eck	Materials Center Leoben Forschung GmbH
08:50	09:10	Tailored inspection intervals for wheelset axles	Jürgen Maierhofer	Materials Center Leoben Forschung GmbH
09:10	09:30	Overview of condition-based wheelset maintenance of rail vehicles at ÖBB	Philipp Linzbichler	ÖBB-Personenverkehr AG
09:30	09:50	Predictive maintenance in reality. An example of optimised wheelset maintenance at SBB	Wilfried Bürzle	SBB AG
09:50	10:20	Coffee break		
start	end	Digitalization and reliability of railway vehicles and tracks II		
10:20	10:40	Initiatives of digitalization for wheel-rail contact studies in Brazil	Professor Roberto Martins de Souza	Universita Sao Paulo, Brazil
10:40	11:00	Rail vehicles in the future: challenges and answers	Thomas Moshhammer, Bernhard Girstmair	SIEMENS-Mobility GmbH
11:00	11:20	Steel development for railway turnouts	Michael Mayer	Materials Center Leoben Forschung GmbH
11:20	11:40	Investigation of the wheel impact load and transition point on fixed crossings, combining MBS & FEA with in-track measurements	Thomas Titze	voestalpine Railway Systems

Friday, 7.6.2024 - Erzherzog Johann Hall

start	end	High-end material characterization methods		
13:00	13:20	Highlights & Challenges of residual stress measurements with electron microscopy	Bernhard Sartory	Materials Center Leoben Forschung GmbH
13:20	13:40	Unprecedented insights into synthesis - structure - property relations of TiSiN coatings by combining advanced characterization techniques	Nina Schalk	Montanuniversität Leoben - Department of Materials Science
13:40	14:00	Towards understanding high-temperature fatigue of WC-Co hard metals via eddy current heated uniaxial loading tests in vacuum	Thomas Klünsner	Materials Center Leoben Forschung GmbH
14:00	14:20	Miniaturized in situ fracture experiments to probe local interface reliability	Daniel Kiener	Montanuniversität Leoben - Department of Materials Science
14:20	14:50	Coffee break		
start	end	Condition monitoring and condition-based maintenance II		
14:50	15:10	The Rayleigh-Ritz Autoencoder – A new method for constructing hybrid models guaranteeing physics constraints	Dimitar Ninevski	Montanuniversität Leoben - Chair of Automation and Measurement
15:10	15:30	Strategies for condition monitoring in drilling production	Tamara Feil	CERATIZIT Austria
15:30	15:50	Condition monitoring for milling tools with reduced instrumentation requirements	Elias Jan Hagendorfer	Materials Center Leoben Forschung GmbH

Friday, 7.6.2024 - Peter Tunner Hall

start	end	Electrical energy storage and conversion I		
08:30	08:50	New Materials for energy storage and energy conversion – an industrial view	Markus Puff	TDK Electronics
08:50	09:10	Analytical and high-resolution electron microscopy of materials for batteries and solar cells	Daniel Knez	TU Graz - Institute of Electron Microscopy and Nanoanalysis (FELMI)
09:10	09:30	Functional coatings for the production of renewable hydrogen	Stephan Abermann	AIT Austrian Institute of Technology GmbH
09:30	09:50	How Artificial Intelligence fosters the Understanding of the Structure Property Relationship in Materials for Energy storage and Conversion Applications?	Roland Brunner	Materials Center Leoben Forschung GmbH
09:50	10:20	Coffee break		
start	end	Electrical energy storage and conversion II		
10:20	10:40	Nanostructured charge transfer layers for perovskite solar cells: an opportunity or a distraction?	Vilko Mandic	University of Zagreb - Department of Inorganic Chemical Technology and Non-Metals
10:40	11:00	Towards green solvent processing of organic solar cells and modules	Thomas Rath	TU Graz - Institute for Chemistry and Technology of Materials (ICTM)
11:00	11:20	Eco- friendly low-cost methods for manufacturing multi-layer thin film capacitors	Ivana Panzic	Materials Center Leoben Forschung GmbH
11:20	11:40	Using effective Hamiltonians to optimize BaTiO ₃ -based ferroelectric materials for capacitor applications	Maxim N. Popov, Florian Mayer	Materials Center Leoben Forschung GmbH

Friday, 7.6.2024 - Peter Tunner Hall

start	end	Reliability of electronic-based systems I		
13:00	13:20	Application of machine learning algorithms for defect analysis in semiconductors using high resolved scanning acoustic microscopy	Peter Czurratis	PVA TePla AG
13:20	13:40	Thermal analysis of innovative vertical GaN based power devices	Sandra Fischer	Materials Center Leoben Forschung GmbH
13:40	14:00	Advanced Characterization and Modeling Needs for Metallizations in Microelectronics Applications	Peter Imrich	KAI
14:00	14:20	Fatigue mechanisms in sustainable solder balls: An ML-assisted, correlative study	Charlotte Cui	Materials Center Leoben Forschung GmbH
14:20	14:50	Lunch		
start	end	Reliability of electronic-based systems II		
14:50	15:10	Challenges in digital light printing of electronic based systems – process development and reliability simulation	Peter Fuchs	Polymer Competence Center Leoben GmbH (PCCL)
15:10	15:30	Thermomechanical coupling of phase transformations and constitutive laws to describe microstructural evolution and fatigue in sustainable solders	Wolfgang Flachberger	Materials Center Leoben Forschung GmbH
15:30	15:50	Process and defect modelling of sapphire crystal growth - track to virtual methodology	Georg Reiss	Materials Center Leoben Forschung GmbH

Organising committee:

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