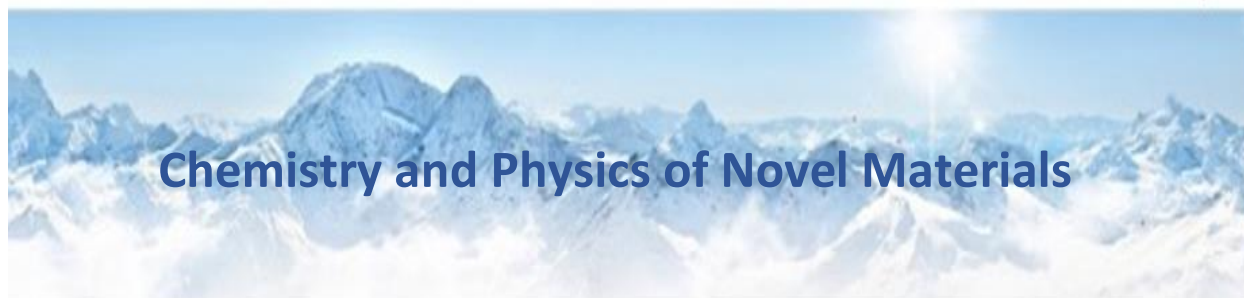




TECHNISCHE  
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## Program of the 37<sup>th</sup> Workshop on



## Chemistry and Physics of Novel Materials

**JUFA Schladming**  
**February 04 - 09, 2024**

<b>Location</b>	JUFA Hotel Schladming Coburgstrasse 253, A – 8970 Schladming Tel: +43(0) 5/7083-330 Fax: +43(0) 5/7083-331
<b>Dates</b>	Arrival: Sunday, February 4 <sup>th</sup> , 2024 (Dinner 18:00, Get Together 20:00) Departure: Friday, February 9 <sup>th</sup> , 2024
<b>Organizers:</b>	<b>Univ.Prof. Dr. Günther Rupprechter</b> <b>Ao.Univ.Prof.Dr. Peter Blaha</b> Institute of Materials Chemistry TU Wien, Getreidemarkt 9/E165, A-1060 Vienna Tel: +43 (1) 58801-165101 E-Mail: guenther.rupprechter@tuwien.ac.at

### Program Committee

B. Batlogg  
F. Gießibl  
G. Rupprechter

P. Blaha  
J. Kunze-Liebhäuser  
K. Schwarz

U. Diebold  
A. Pimenov  
P. Weinberger

<https://www.tuwien.at/tch/imc/konferenzen/37th-workshop-on-chemistry-and-physics-of-novel-materials>

## Scientific Program

**Monday, Feb. 5<sup>th</sup>, 2024**

**Surface Science and Catalysis, powered by MECS®**

Chair: Günther Rupprechter (TUW)

**14:00** Opening 37<sup>th</sup> Workshop

**14:05** Introduction

**14:20** Dominik Eder (TUW)

Metal-organic frameworks as next-generation photocatalyst

**15:00** Coffee Break

**15:30** Jörg Libuda (Univ. Erlangen)

Atomic Layer Deposition of semiconductor films on functionalized oxides:  
in-situ studies in ultrahigh vacuum and in liquid environment

**16:10** Christophe Copèret (ETH Zurich)

(NMR) Centered on Metals

**16:40** End

**18:00** Dinner

Evening Session: Chair: Aleix Comas-Vives (TUW)

**19:30** Philipp Winkler (TUW)

How in situ correlative microscopy can image interface and particle size effects in catalytic reactions

**20:00** Shun Kashiwaya (Linköping University)

Single-atom-thick sheets of gold—goldene—and perspectives in their potential application

**20:30** End

**For all talks leave 5-10 min discussion time !!**

**Tuesday, Feb. 6<sup>th</sup>, 2024**

## **MECS: Episode II**

Chair: Alexander Genest (TUW)

- 14:00 Konstantin M. Neyman (ICREA & Univ. Barcelona)**  
Quantifying interface effects in catalytic nanomaterials combining DFT modelling and experiments
- 14:40 Alexey Cherevan (TUW)**  
Molecular polyoxo- and thiometalate clusters as a bridge between homogeneous and heterogeneous photocatalysis
- 15:10 Coffee Break**
- 15:30 Introduction: Peter Weinberger (TUW)**
- 15:45 Birgit Weber (Friedrich-Schiller-Universität Jena)**  
Switchable spin states in the city of light
- 16:25 End**

**18:00 Dinner**

## **Highlights in Advanced Coordination and Metal-organic Chemistry**

Evening Session: Chair: Peter Weinberger (TUW)

- 19:30 Grace Morgan (University College Dublin)**  
Spin-state switching in non-centrosymmetric crystals
- 20:00 Martin Huber (TUW)**  
Spin switching luminescent Fe(II) tetrazole-BODIPY complexes
- 20:30 End**

**For all talks leave 5-10 min discussion time !!**

**Wednesday, Feb. 7<sup>th</sup>, 2024**

## **Topologically Nontrivial Materials**

Chair: **Andrei Pimenov** (TUW)

- 14:00** Introduction to Topology and Magnetism (Andrei Pimenov)
- 14:20** **Florian Libisch** (TUW)  
Quantum Hall edge states using Scanning Tunneling Microscopy
- 14:55** **Coffee Break**
- 15:25** **Ekaterina Pomjakushina** (PSI Villigen)  
Crystal growth and physical properties of crystals with topological magnetic phases
- 16:00** **Vladimir Pomjakushin** (PSI Villigen)  
Topological magnetic structures in MnGe and CeAlGe: Neutron diffraction and symmetry analysis
- 16:35** **End**

**For all talks: 5-10 min discussion suggested !!**

**18:00** **Dinner**

Evening Session: Chair: Peter Blaha (TUW)

- 19:00** **Meeting of the Program Committee**
- 19:30** **Poster short presentations and poster session**

Please prepare a 3 minutes poster presentation (max 3 slides !) and send it to [peter.blaha@tuwien.ac.at](mailto:peter.blaha@tuwien.ac.at)

**Thursday, Feb. 8<sup>th</sup>, 2024**

**New Faces at the TU Wien**

Chair: **Andrei Pimenov** (TUW)

- 14:00** Introduction to modern magnetism
- 14:10** **Marta Gibert** (TUW)  
Magnetic double-perovskite oxide heterostructures
- 14:45** **Coffee Break**
- 15:15** **Amalio Fernández-Pacheco** (TUW)  
3D magnetic nanomaterials for computing applications
- 15:50** **Andrej Pustogow** (TUW)  
New Spin on Electrons in Solids: Stress Reduces Frustration
- 16:25** **Philipp Haslinger** (TUW)  
Electron spin resonance meets electron microscopy
- 17:00** **End**

**18:00** **Dinner**

Evening Session: Chair: Peter Weinberger, Science Busters

- 19:30** **Bertram Batlogg** (ETH Zurich)  
Technology: never enough?
- 20:15** **Anna Pimenov** (TUW)  
Old Art – New Science
- 20:45** **End**

**For all talks leave 5-10 min discussion time !!**

**Friday, Feb. 9<sup>th</sup>, 2024**

**Sci-Mix**

Chair: Johannes Zeininger (TUW)

**14:00 Xiaoyu Zhou** (ETH Zürich)

Small cobalt nanoparticles favor reverse water-gas shift reaction over methanation under CO<sub>2</sub> hydrogenation conditions

**14:30 Aleix Comas-Vives** (TUW)

Modelling the nature and dynamics of active sites in heterogeneous catalysts

**15:00 Camilla Codeço** (Federal University of Rio de Janeiro)

Insights into the reactivity of Mn<sub>3</sub>O<sub>4</sub> (001) thin films with water

**15:30 Closing Remarks**

**16:00 End**

**For all talks leave 5-10 min discussion time !!**

## POSTER CONTRIBUTIONS

Investigation of magnetic states in multilayers with chiral interlayer interactions

M. Á. Cascales Sandoval

Exploring the synergies of gamma alumina and tutton salt hydrates in thermochemical energy storage

J. Smith, J. Werner, F. M. Kapsamer, A. Ristić, A. Werner, P. Weinberger

Miniaturized Mössbauer spectrometer mimos: Selected by esa for a moon mission

F. Renz, F.-W. Bauer, J. Pawlak, M. Beyki, R. Lucka, R. Gieseler, K. Tran, M. S. Kilic, M. Linnemann, M. Smajlaj, A. Sander, J. Brehme, L. Renz, M. Renz, H. Gaber, R. F. Sindelar, D., R. Patzke, C. Rajnák, R. Boča

Single particle catalysis

J. Zeininger, M. Raab, G. Rupprechter

Harnessing low-grade heat for sustainable power generation: advancing materials and beyond

F. M. Kapsamer, J. Smith, J. Werner, A. Werner, P. Weinberge

Calcium dicarboxylate salt hydrates as thermochemical energy storage materials for household applications

J. Werner, J. Smith, A. Werner, P. Weinberger

Research on new potential materials for thermochemical energy storage : Alums and composite materials

A. Larchier, J. Smith, A. Ristic, P. Weinberger

Sodium nanoparticle adsorption on magnesium oxide surface using full potential plane wave methods

R. Mohammad, A. Elashqar

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### General Information:

Breakfast: 07.00 – 10.30

Dinner: 18.00 – 19.00