MAX-PLANCK-INSTITUT
FÜR CHEMISCHE ENERGIEKONVERSION

EPR for Catalysis Research

An international workshop on the application of EPR spectroscopy in catalysis and on the role of electron spin in catalytic processes

10th–13th September 2023, Schloss Ringberg, Kreuth-Reitrain, Germany

Welcome note

The organizing committee welcome you at the “Electron Paramagnetic Resonance for catalysis research” workshop.

Workshop topics include in situ and spectro-electrochemical EPR, magnetic-structural correlations, spin- and magnetic-field-dependent catalysis, combined EPR and NMR approaches, and EPR on catalytic coordination complexes and solid-state materials/electrodes. The aim of the workshop is to allow intensive discussions and

exchange across the different disciplines of catalysis. In this respect, the program was formed on the basis of invited scientists based on their significant contribution in the field.

We wish to thank the Max-Planck Society for allowing us to exploit the beautiful location of Schloss Ringberg for this workshop with its excellent conference infrastructure and the Ernst-Rudolf-Schloeßmann Stiftung for funds to support participants from Max Planck Institutes and the Max Planck Institute for Chemical Energy Conversion for additional funding and administrative support. Welcome and enjoy your staying in the Ringberg castle!

Schloss Ringberg, September 2023

Alexander Schnegg and Paolo Cleto Bruzzese

Organizing Committee

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General Information for the participants

Travel Information

By plane

From Munich Airport (MUC), take the S-Bahn line S1 or S8 to Munich Central Station. Continuation to Tegernsee station: distance 59 km (final station), travel time approx. 1 hour. For details see *By train*.

By train

To Munich central station by Deutsche Bahn - onward journey to Tegernsee station: distance 59 km (final station), journey time approx. 1 hour. Details see timetable (Bayerische Oberlandbahn BOB). From the station we recommend using a taxi: e.g. Taxi Jasinski Tel. +49 (0)8022 / 95 0 99.

By car

Motorway Munich-Salzburg A8 (E45) via motorway junction Brunnthal to exit 97 Holzkirchen. Continue on the B318 to Gmund am Tegernsee. In Gmund turn off to Bad Wiessee and continue to the traffic lights after the town sign of Weißach. Here turn right into the federal road B307 towards Achensee. After approx. 1 km drive off the federal road B307 shortly after the end of Reitrain and continue straight on for approx. 100 m until the specially signposted access avenue at the edge of the forest (1.8 km gravel road with 9% gradient) to Ringberg Castle.

Important note!

The organizers will arrange a shuttle mini-bus for helping to pick up the participants from Tegernsee train station up to the Ringberg Castle. Please inform in advance the organizing committee about the arrival time at the Tegernsee station.

Timetable EPR for Catalysis Research workshop, Ringberg 10th-13th September 2023

Time\Day	Sunday 10th	Monday 11th	Tuesday 12th	Wednesday 13th
7:30 – 9:00		Breakfast	Breakfast	Breakfast
9:00 – 9:35		**SSM 1** Mario Chiesa	**IS/SEC 1** Damien Murphy	**CC 1** Piotr Pietrzyk
9:35 – 10:10		**SSM 2** Paolo Cleto Bruzzese	**IS/SEC 2** Angelika Brückner	**CC 2** Karsten Meyer
10:10 – 10:45		**SMM 3** Karsten Seidel	**IS/SEC 3** Jean Ansermet	**CC 3** Emma Richards
10:45 – 11:15		Coffee break	Coffee break	Coffee break
11:15 – 11:50		**SSM 4** Andreas Pöppl	**IS/SEC 4** Maxie Rössler	**CC 4** Ivana Ivanovic-Burmazovic
11:50 – 12:25		Lunch	**IS/SEC 5** Silvio Künster	**CC 5** George Cutsail
12:25 – 13:45			Lunch boxes	Optional Lunch boxes
13:45 – 14:20		**ES/A 1** Vera Krewald	**Long break for walking**	
14:20 – 14:55		**ES/A 2** Thomas Lohmiller		
14:55 – 15:30		**ES/A 3** Shengfa Ye		
15:30 – 16:00	**Opening\Arrival**	Coffe break		
16:00 – 16:35	**(Posters setting)**	**ES/A 4** Dana Dvoranova	**HR 1** Thomas Wiegand	
16:35 – 17:10		**ES/A 5** Daniel Klose	**HR 2** Gunnar Jeschke	
17:10 – 17:45		**ES/A 6** Christoph Coperet	**HR 3** Edward Reijerse	
17:45 – 18:20		**Castle Tour**	**HR 4** Müge Kasanmascheff	
18:20 – 19:00			Break	
19:00 – 20:00	Dinner	Dinner	Dinner	
20:00 – 20:20	**Welcome**	**COST action meeting / free evening**	**Poster Session (odd numbers)**	
20:20 – 21:00	**Pitch presentations for participants presenting posters**			
21:00 – 22:00			**Poster Session (even numbers)**	

SSM: Solid-state materials for catalysis

ES/A: Electronic Structure/Activity

IS/SEC: In-situ EPR/Spectro-electrochemical EPR

HR: High-resolution EPR for active site characterization

CC: Coordination compounds for small molecule activation

Titles of the talks

- **SSM 1**: *Surface Chemistry and Catalysis by EPR: Concepts, Examples and Perspectives*
- **SSM 2**: *EPR coupled to electronic structure methods for the characterization of active single-metal sites in microporous materials*
- **SSM 3**: *Applications of EPR spectroscopy in chemical industry, with a focus on catalytic materials, and benchtop instrumentation*
- **SSM 4**:

- **ES/A 1**: *Electronic Structure Analyses of Iron Complexes for Electrocatalytic Oxygen Reduction*
- **ES/A 2**: *EPR as a Toolbox for the Characterization of Intermediates in Small Molecule Activation at Transition Metal Centers: Oxygen Activation at Biomimetic Dinuclear Sites and CO_2 Reduction by a Co Complex*
- **ES/A 3**: *Electronic Structures and Reactivity of Iron(V)- Nitrido and -Oxo Complexes*
- **ES/A 4**: *CW-EPR spectroscopy in heterogeneous photocatalysis*
- **ES/A 5**: *Magnetic Resonance (EPR/NMR) to uncover electronic structure of surface species in heterogeneous catalysis*

- **IS/SEC 1**: *Deploying EPR and perturbation methods to study catalytic reactions*
- **IS/SEC 2**: *Opportunities and Limitations of in situ and Operando EPR Spectroscopy in Catalysis*
- **IS/SEC 3**: *Magnetic Resonance Characterization of spin effects at electrodes*

- **IS/SEC 4**: *In situ and operando film-electrochemical EPR as a new tool to investigate 'heterogenised' molecular electrocatalysis*
- **IS/SEC 5**: *EPR-on-a-Chip for Catalysis Research*

- **HR 1**: *Active centers in ATP-fueled motor proteins studied by combining solid-state NMR with EPR spectroscopy*
- **HR 2**: *Identification of active species and mechanisms in catalysis by operando EPR and reaction gas modulation*
- **HR 3**: *Detection of paramagnetic intermediates in Nickel and Bismuth based organo-metallic catalytic systems*
- **HR 4**: *Structure elucidation of a metalloDNAzyme*

- **CC 1**: *EPR insight into coordination and activation of small molecules – toward generation of reactive species on oxide and zeolite catalysts*
- **CC 2**: *Long-lived, ambient Cr(III)-based near-IR emission, and Donor-Acceptor Dyads for Upconversion Technologies*
- **CC 3**: *Bioinorganic redox modulation, catalysis and signaling for medical, environmental and energy applications*
- **CC 4**: *EPR Characterization of Heavy Main Group Radicals*