



EFEPR

18-25/11/2019

CZECH REPUBLIC

Hotel Skalský dvůr



**8th School
of the European
Federation of EPR groups
on Advanced EPR**

www.eprschoo.ceitec.cz



CEITEC

1. ORGANIZERS CEITEC BUT

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Antonín Sojka
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2. SPONSORS

Societies



CEITEC



EFEPR



MOI Spin



GDCh-EGMR



SharedEPR



ARPE



Gropement Ampere



International ERP Society



PETER

Companies



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THz Instruments



FeMi Instruments



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Journals



Springer

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European Journal of Inorganic Chemistry

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3.

WELCOME

Dear Students, Dear Colleagues,

On behalf of the Brno Central European Institute of Technology (CEITEC) and the Magneto-Optical THz Spectroscopy (MOTES) group of the Brno Technical University (BUT), Czech Republic, it is our great pleasure to welcome you to the 8th European Federation of EPR groups (EFEPG) school event on Advanced EPR, held in the Brno region from the 18th to 25th November, 2019 at the Hotel Skalský dvůr.



the only production of its kind in any of the Eastern European countries, and it continued for the next 25 years. During its time, TESLA managed to produce about 500 spectrometers. In 1967 Professor Dadok left for an internship in the USA and did not return after the Soviet occupation of Czechoslovakia in August 1968. In 1976 he became Technical Director of the Pittsburgh National Nuclear Magnetic Resonance Centre and full professor for chemical scientific instruments at the Carnegie Mellon University. In 1977 he completed the development of the first superconducting spectrometer, with a field strength of 14.1 T and working at a frequency of 600 MHz, which remained the most powerful NMR system for high-resolution spectroscopy in the world for a full eight years.

On this occasion I would like to mention the brief history of magnetic resonance in the Czech Republic, and especially its connection to the city of Brno and Josef Dadok. [1,2] Josef Dadok (28.2.1928, Dětmárovice, Czech Republic) is a renowned Czech scientist and innovator: the pioneer of NMR spectroscopy. He graduated from BUT in Brno in the early 50s. He founded The Nuclear Magnetic Resonance Department at the Institute of Scientific Instruments, Czechoslovak Academy of Sciences (ISI) in 1960 and together with his team he developed the first devices for NMR spectroscopy in the Czech Republic. At that time, the US imposed an embargo on the Soviet Union for NMR spectrometers, which was a very unfavorable situation for research in Eastern Bloc states. The Institute of Scientific Instruments was just ten minutes away from the company TESLA Brno. TESLA had a state-sponsored monopoly on electronics production in Czechoslovakia, and produced nearly all electronic products in the country until 1989. Tesla became the manufacturer of Josef Dadok's first 60MHz spectrometer, named TESLA BS477, which was put into production in 1965. Thus, Czechoslovakia became the third country, after the USA and Japan, to succeed in the serial production of these scientific devices. This was

Moreover, Josef Dadok is linked to EPR via Rapid Scan. His paper on correlation spectroscopy in 1973 [3] inspired Sandra and Gareth Eaton to apply this method to EPR. It took a while, but this year, EPR Rapid Scan instruments were commercially released by Bruker at the Rocky Mountain conference in Denver. The legacy of Josef Dadok in Brno is still alive. The National NMR Centre at CEITEC has carried the name of Josef Dadok since 2013. The NMR Centre is equipped with the most powerful NMR spectrometer in Central and Eastern Europe.

My team and I wish to reestablish the tradition of magnetic resonance development in Brno started by Josef Dadok. In conclusion, we believe that you will enjoy the school and we, the local organizing committee, are looking forward to an exciting EPR school event!

Petr Neugebauer
On behalf of organizers

[1] B. Král and A. Blatná, *Slaboproudý obzor*, 72, 4 (2016)

[2] V. Zeman, *Vzpomínky na NMR v Brněnské Tesle*. Stan's Library: http://www.ebyte.it/library/hist/NMR_Tesla_cs.html. ISSN 2421-1230.

[3] J. Dadok and R.F. Sprecher, *Correlation NMR spectroscopy*. *J. Magn. Reson.* 13, 243 (1974).

4.

PRACTICAL INFORMATION

Badges

Organizer

Speaker

Participant

WIFI

Login: FreeSD
Password: skalskydvur

Hotel rooms
Login: ap-hotel
Password: no password

Contacts



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petr.neugebauer@ceitec.vutbr.cz

Emergency Line 112
Emergency Medical Service 155
Fire Brigade 150
Municipal Police 156
National Police 158

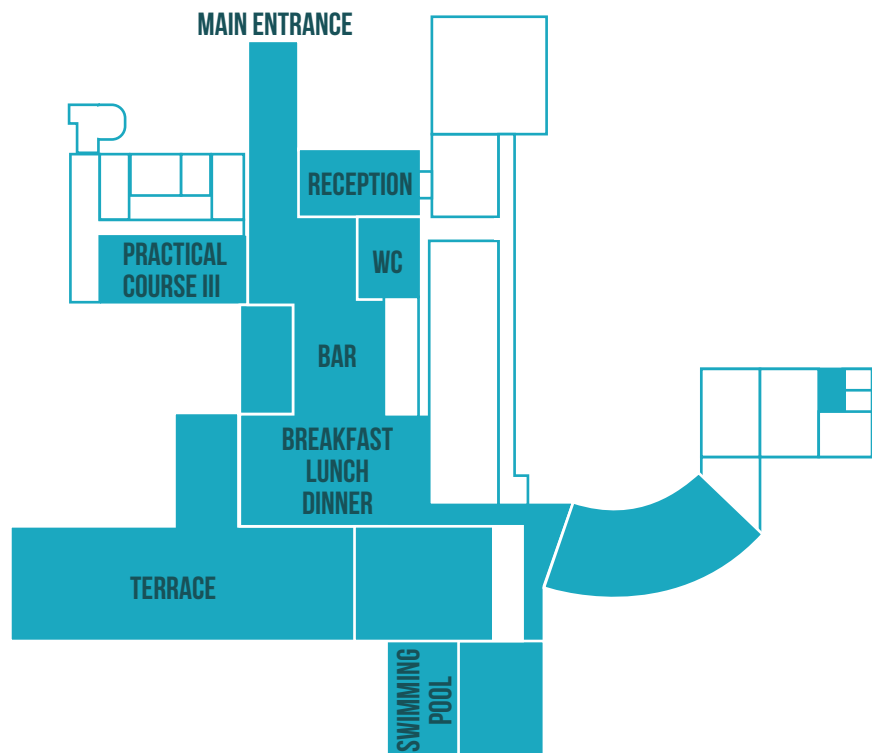


Lenka Honková

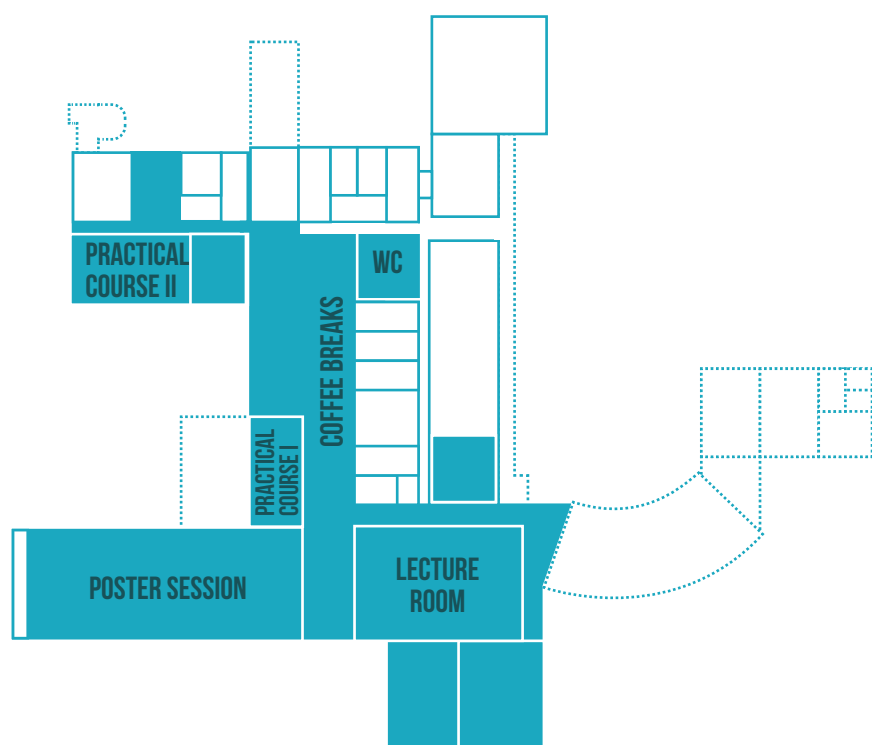
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eprschool@ceitec.vutbr.cz

HOTEL SKALSKÝ DVŮR PLAN

Ground floor



Underground floor



TIPS FOR TRIPS

Pernštejn
castle



UNESCO Pilgrimage
Church of St John of
Nepomuk at Zelená Hora



Ždár nad
Sázavou
castle



Eden Centre
an educational farm
Bystrice nad Pernštejnem



Glassworks
Škrdlovice



Nové Město Na
Moravě
sport Arena Vysočina



Polička
historical town

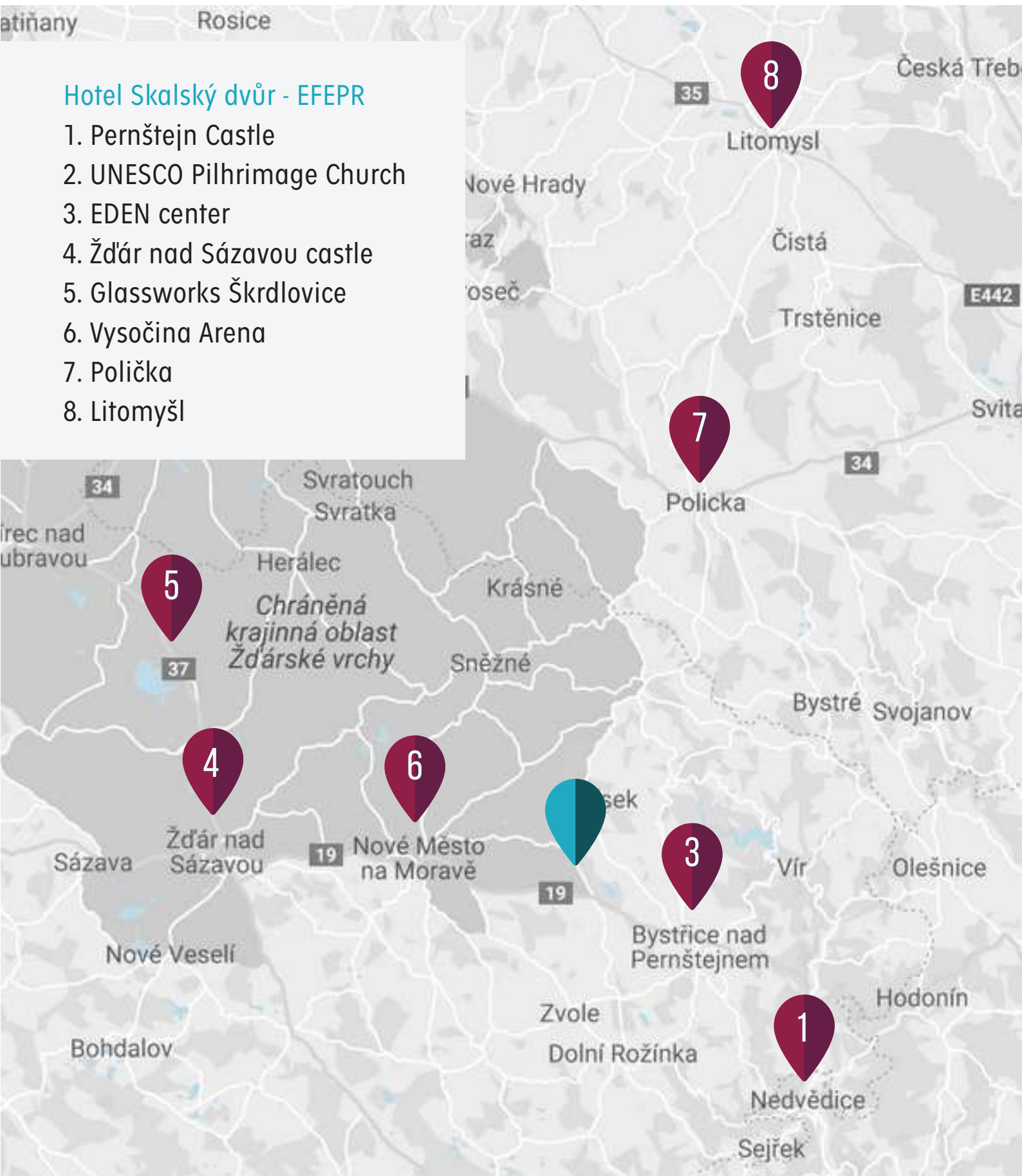


Litomyšl
historical town
and castle



Hotel Skalský dvůr - EFEPR

1. Pernštejn Castle
2. UNESCO Pilgrimage Church
3. EDEN center
4. Žďár nad Sázavou castle
5. Glassworks Škrdlovice
6. Vysočina Arena
7. Polička
8. Litomyšl



5. SPONSORS



high performance electron paramagnetic resonance spectrometer

Bench-top ESR spectrometer MiniScope MS 5000

Highlights

- Cost efficient
- Compact size
- High sensitivity
- Outstanding magnetic field stability
- Wide range of accessories and glassware

Wide field of application

- Alanine dosimetry
- Medical research
- NO measurements
- Food safety and quality
- Separation of radicals
- Beer analysis
- Environmental toxicology
- Bioinorganic chemistry
- Petro chemistry



Accessories

- Liquid nitrogen thermostat: temperature range 93 – 473K
- Flow-through-system for kinetic measurements
- Autosampler
- Software: automatic data acquisition and data calculation
- Glassware: flat cells, tissue cells, dewars, etc.

Technical data

- Sensitivity: 5×10^9 spins/0.1 mT
- Scan range: 0 – 625 mT
- Magnetic field range: 0 – 650 mT
- Modulation frequency: 10 kHz and 100 kHz



Kinetic of ROS generation by xanthine/xanthine oxidase



Basal (black) and stimulated (blue) NO generation by rat aorta



TEMPOL in a two phase system oil/water



Spectrum of an Alanine tablet irradiated with 5 Gy



Thomas Keating Ltd

2 GHz to >3 THz

www.terahertz.co.uk



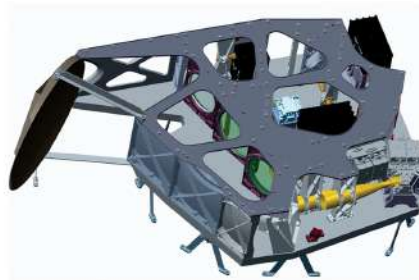
Design and manufacture of Microwave, Millimetre wave and Terahertz Quasi-Optical systems for space and terrestrial application in cosmology, astronomy, remote sensing, materials measurements and structural biology

MIT/NASA TROPICS



CubeSat Antennas

EUMETSAT MicroWave Sounder MetOp-SG



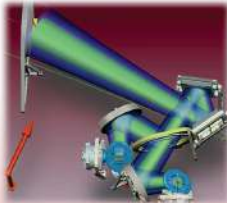
23 - 229 GHz
Quasi Optic Network

HiPER 94 GHz ESR



Electron Spin Resonance
Quasi Optics

JAXA'S EarthCARE



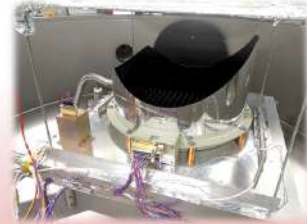
CAD Design
of 94 GHz
CPR Radar

ESA's Cosmic Background PLANCK



Space qualified
corrugated horns

Radiometer PRT Calibration



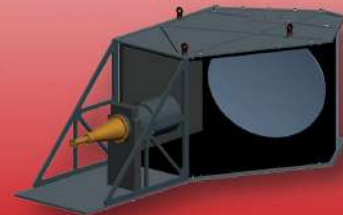
Using In-house TVAC

JAXA's JEM/SMILES



640 GHz Quasi Optics

Antennas



12-18 GHz for material measurement

- Radar Absorbing Materials
- TVAC in clean room
- HFSS & GRASP analysis
- QO Analysis in CAD
- Integrated CAD/CAM
- Electroforming
- CNC Machining
- Spark Erosion
- CMM Inspection



Electroforming

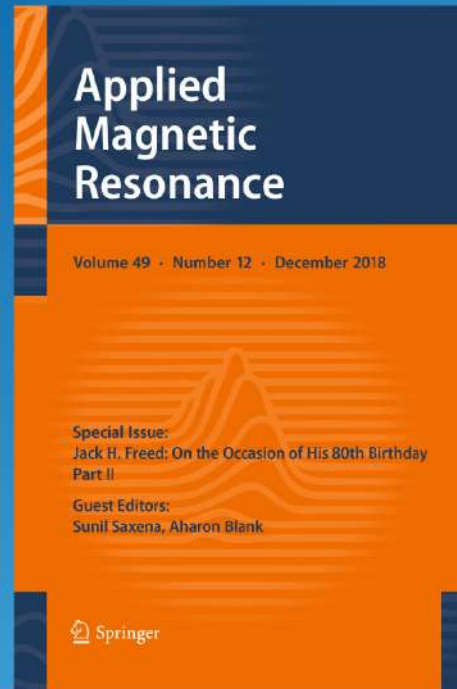


TVAC in a Cleanroom

Editor-in-Chief:
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ISSN 1613-7507 (electronic version)



Applied Magnetic Resonance provides an international forum for the application of magnetic resonance in physics, chemistry, biology, medicine, geochemistry, ecology, engineering, and related fields.

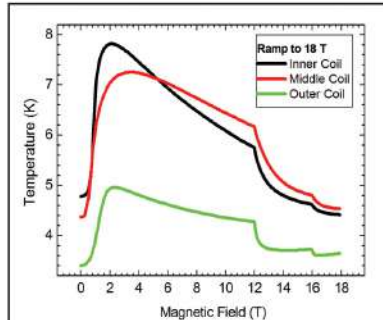
The contents include articles with a strong emphasis on new applications, and on new experimental methods.



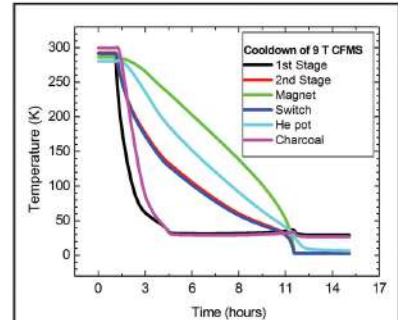
CRYOGEN-FREE MEASUREMENT SYSTEMS TO 18 TESLA



18 T cryogen-free measurement system with rotating system with ^3He insert



Ramp of magnetic field to 18 T showing the temperatures of the coils and magnetic field during the ramp



Typical cooldown graph of 9 T cryogen-free system



New Upgraded VSM Model

9 T mini cryogen-free measurement system with VSM insert



- Magnetic fields from 3 T to 18 T
- 1.6 K to 400 K as standard
- mK stability across the temperature range
- 50 mK to 1000 K available with special options
- 20 bit power supply provides precise field control

Benefits of the Cryogen-Free System

- Low operating costs with very long maintenance interval
- Automated and easy to use
- Modular architecture allows many different measurement inserts
- No special cryogenic experience required

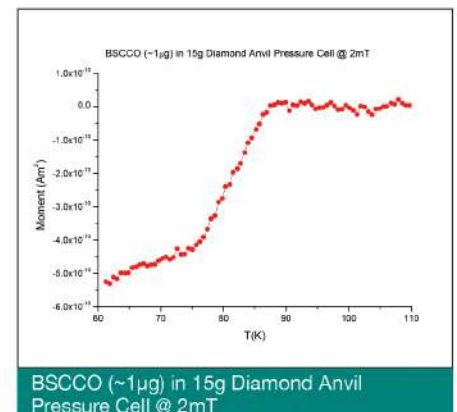
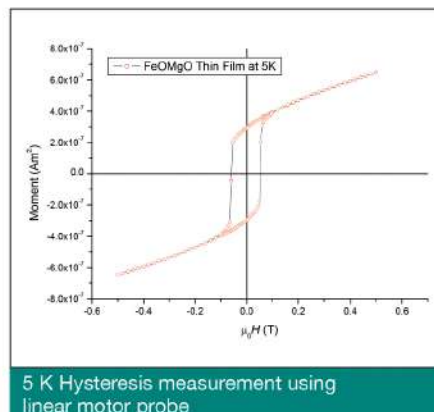
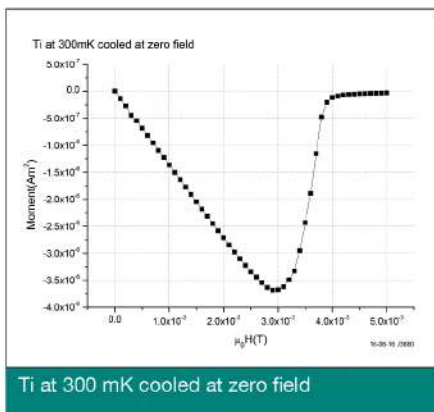
HIGH SENSITIVITY SQUID MAGNETOMETER WITH He-3 PROBE FOR TEMPERATURES DOWN TO 300 mK



- Fast scan Linear Motor (LM) Facility
- Higher resolution
- Requiring no liquid helium refills
- Cryocooled 7 Tesla SQUID system
- Zero boil-off
- AC and DC measurements with 10^{-8} EMU sensitivity
- Smooth transition across 4.2 K
- Real-time data access during measurement
- MilliTesla field resolution and setting
- Low maintenance pulse tube cryocooler
- Flexible open LabVIEW® software

Options

- He-3 Insert for temperatures down to 300 mK
- High temperature facility
- Electrical resistivity measurements
- Horizontal sample rotator
- Ultra low field
- Fibre optic probe





The Rapid Scan accessory comprises the following components :

- | | |
|----------------------------------|---------------------------|
| 1. RS Driver | 5. RS Coils |
| 2. RS Acquisition Unit | 6. Water cooler for coils |
| 3. RS Resonator | 7. Capacitor unit |
| 4. MW Frontend with I/Q Detector | |

A Revolution in EPR - Introducing the Rapid Scan Accessory

RS-EPR is a revolutionary technique that opens new possibilities not previously available with conventional CW-EPR. With an increase in the signal to noise ratio and a decrease in the acquisition time, RS-EPR can probe very low concentrations and very fast reactions.

- Field scan width: up to 200 G per segment
- Field scan times: as low as 10 microseconds
- Compatible with EMXplus and ELEXSYS (10" magnet)
- Compatible with all variable temperature accessories

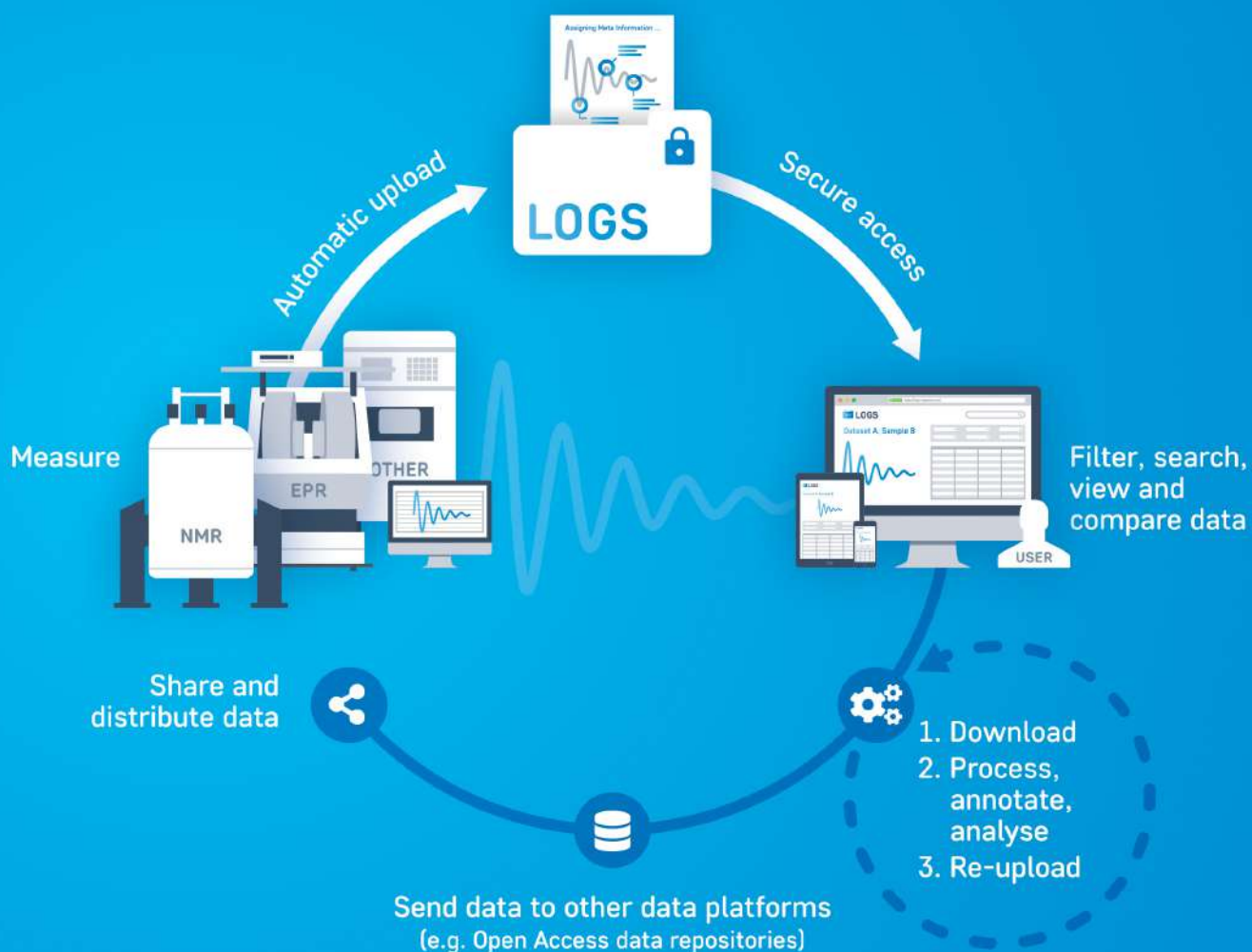
Innovation with Integrity

EPR





LOGS


The **SIGNALS** data repository




The LOGS Editions

 LOGS for service facilities

 LOGS for academia

 LOGS for enterprises

 LOGS for education

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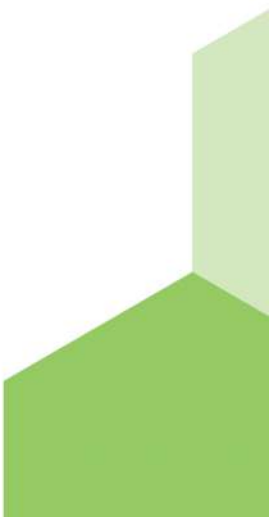
SIGNALS | FiZ - Frankfurt Innovation Center | Altenhöfer Allee 3 | 60438 Frankfurt am Main, Germany



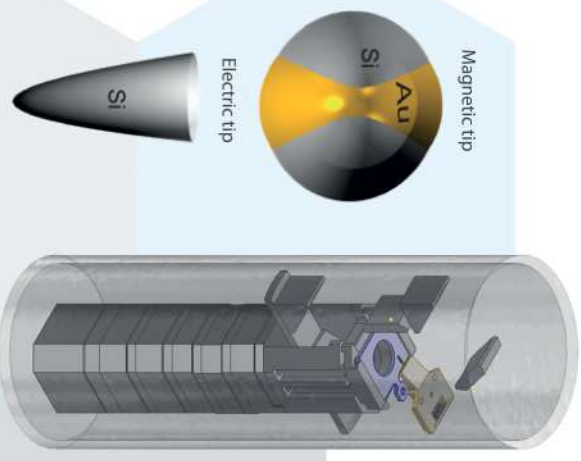
The PETER concept proposes a qualitatively new approach into the EPR area. It builds upon the strong enhancement and subwavelength spatial resolution of magnetic sensing field provided by plasmonic effects based on collective oscillations of electrons at surfaces or in nanostructures.

In contrast to usual THz plasmon-enhanced spectroscopy of nonmagnetic materials, we build upon magnetic plasmonic resonances. This presents unprecedented implementation of plasmonic phenomena into EPR technique. In particular, our project introduces for the first time plasmonic effects into THz EPR.

Combining Electron Spin Paramagnetic Resonance (EPR) with Atomic Force Microscopy (AFM) and plasmonic resonators, the cumulative instrument from the PETER project will provide a step change in the measurement of local materials properties— both solid state (such as magnetic materials used in computer memory) and biological (such as cell wall proteins) – that contain unpaired electrons. This instrument will enable terahertz (THz) (200 GHz – 1 THz) EPR microscopy and spectroscopy at high magnetic fields (12T) and cryogenic temperatures (10 K) with 1 µm or better image resolution. THz EPR microscopy under such conditions has never been done before. The local enhancement of the field via plasmonic resonators to enhance the EPR signals is another component of this instrument that has not been done



previously. This instrument will combine multiple novel techniques in order to locally detect the EPR signal, which can have significant impact in detecting defects in the manufacture of hard drives and RAM for computing as well as detecting variations in the distribution of radical containing proteins in tissue/cell samples for diagnoses and disease pathway analyses. Example biological systems that could be studied by this technique include hem-proteins for blood-based disease analysis and proteorhodopsin (proton-pumps) incorporated in functional materials.



PLASMON ENHANCED TERAHERTZ ELECTRON PARAMAGNETIC RESONANCE

Horizon 2020 project FET OPEN



Project Outcomes

- » Establishing a **brand novel** terahertz-frequency EPR/micro-spectroscopic **technique** based on a combination of **plasmonic** based **magnetic field enhancement** and **scanning probe microscopy**.
- » **Developed THz EPR micro-spectroscope** will offer unprecedented **sensitivity** (several orders higher than conventional EPR instruments) and **spatial resolution below 1 µm** (approx. 1/300th of used wavelength).

Why all the fuss?

If successful, PE THz EPR micro-spectroscopy will mean a revolution in the field of EPR by opening new possibilities to in-situ study of wide variety of materials for scientific, technological and medical purposes.



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Pulchryova 123
612 00 Brno
+420 778 11 4 038
info@peter-
instruments.eu
www.peter-instruments.eu

This project has received funding from the European Union's Research and Innovation Programme Horizon 2020 under Grant Agreement No. 767227.



VAKUOVÁ TECHNIKA

✓ PRŮMYSL ✓ LABORATOŘE ✓ R&D

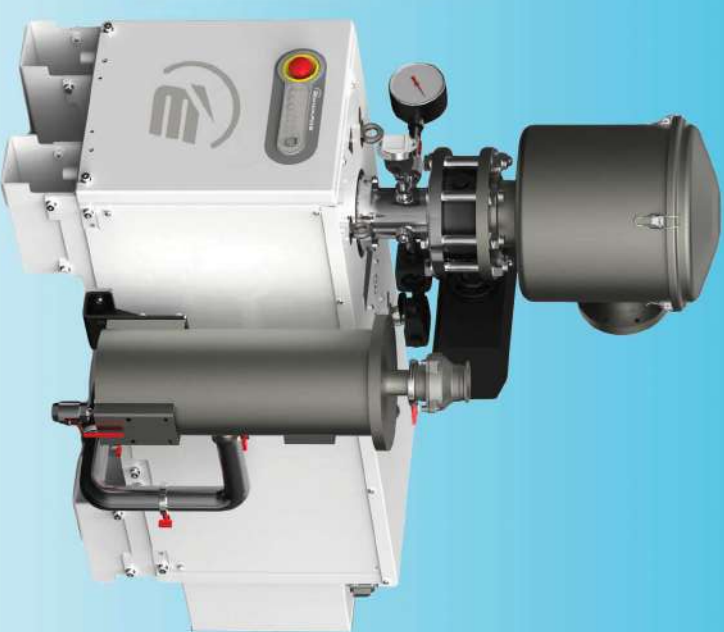
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www.edwardsvacuum.com

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- ✓ SERVIS 24 / 7
- ✓ MODERNIZACE
- ✓ INSTALACE
- ✓ PROJEKCE
- ✓ MĚŘENÍ A KALIBRACE
- ✓ VÝZKUM A VÝVOJ



Turbo-molekulární vývěva nEXT
(výroba a vývoj v ČR)



Suchoběžný čerpací systém 4. generace GXS
(až 5 let bez nutnosti servisu, vyrobeno v ČR)

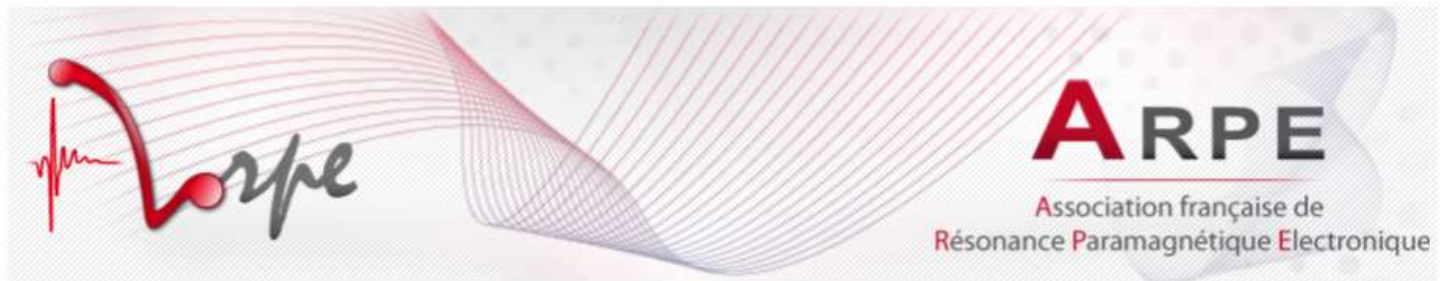


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SK: Activair SK s.r.o. | Cementárenská cesta 16. 974 01 Banská Bystrica



ARPE is the French association dedicated to the French EPR community. Since its creation in 2004, the association has organized annual scientific meetings and schools every two years. Its main objectives are : (i) to stimulate the development of electronic paramagnetic resonance in France , (ii) to participate in the training at the RPE by the organization of schools, workshops, seminars, (iii) to contribute to the development of the areas of application of the EPR and (iv) to promote scientific and technical exchange, contacts between users represent the discipline at the national and international levels.

For the young EPR researchers, ARPE awards every year a thesis prize and a poster prize during the annual scientific meeting and provides grants to participate to EPR international conferences and schools.

All informations are available at <http://www.a-rpe.fr>.

Carole Duboc, Chair of ARPE

BRIDGE

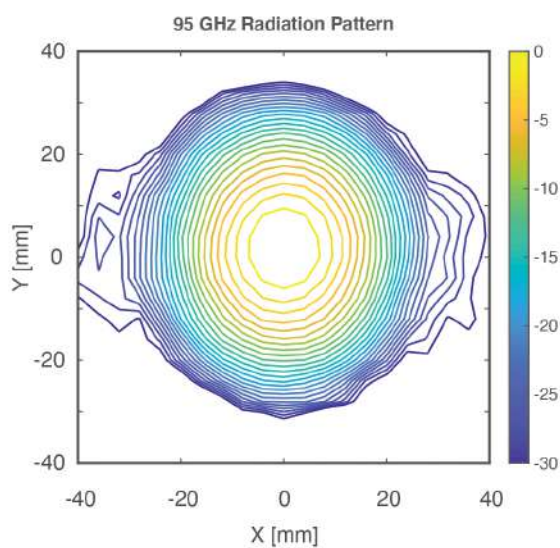
12

Focus on Your Research,
Not Building Instrumentation.

- High-Field EPR/DNP Spectrometers
- Instrumentation for Overhauser DNP
- Gyrotrons for DNP Spectroscopy
- THz Diagnostic Tools
- Gaussian Beam Quasi-Optics
- Corrugated Waveguides, Horns and Tapers



Corrugated 95 GHz HE_{11} Launcher
for High-Field EPR Spectroscopy



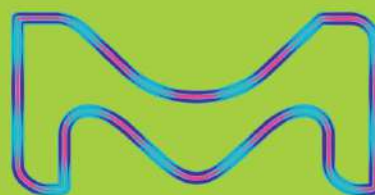
TAKING SCIENCE

Further Faster

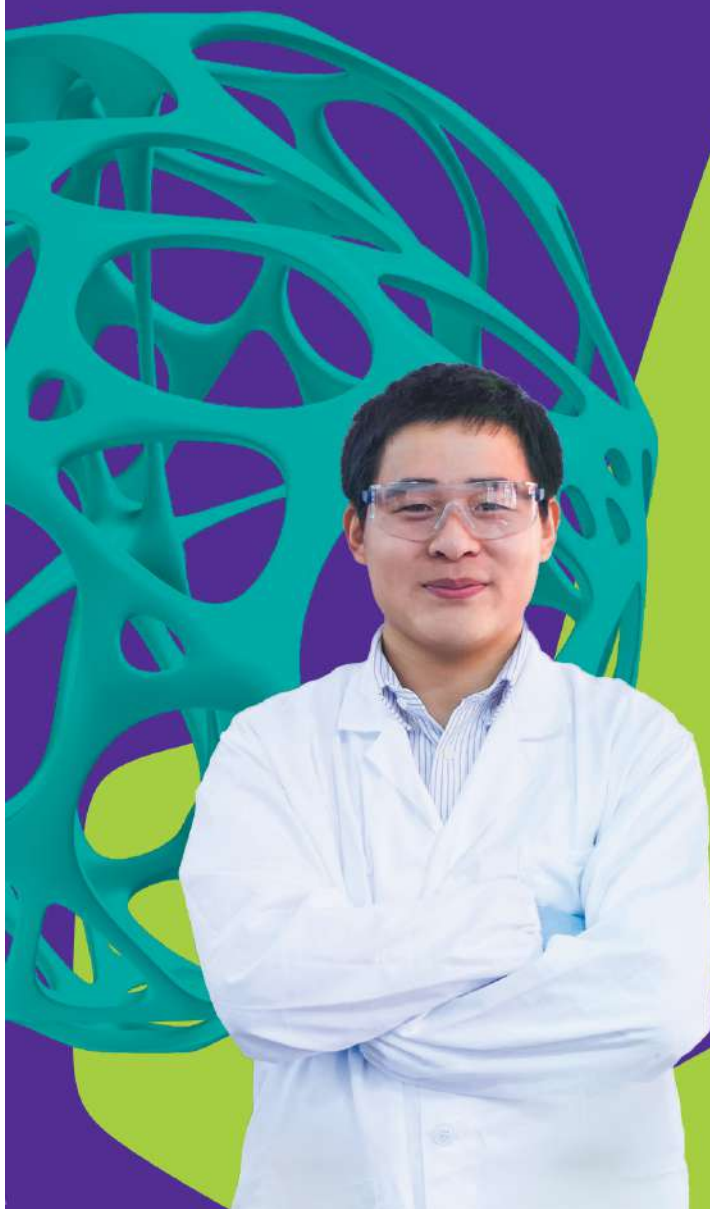
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- Greater investment in innovations

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sigmaaldrich.com



MERCK



Glacios and Falcon 3EC for cryo-EM single particle analysis

Proven technology for fast 3D structures



The Thermo Scientific™ Glacios™ Cryo-TEM allows for sample screening and data acquisition for single particle analysis (SPA). Together with the embedded Thermo Scientific Falcon™ 3EC direct electron detector, the combination provides access to cryo-electron microscopy (cryo-EM) with improved ease-of-use and high level automation – all within a footprint that fits any lab.

Find out more at thermofisher.com/EM-Sales

ThermoFisher
SCIENTIFIC



Virginia Diodes, Inc.
virginiadiodes.com



Transmit and Receive Systems Covering the 70GHz-3THz Spectrum

VDI offers a wide variety of transmit and receive systems covering the 70GHz-3THz spectrum. These systems incorporate VDI's frequency extension and mixer components coupled with commercially available microwave oscillators and amplifiers.

For transmit systems, VDI can configure them with or without a drive oscillator. A VDI Amplifier / Multiplier Chain (AMC) requires a customer supplied low frequency source (typically <20GHz, 10dBm nominal). A VDI Transmitter (Tx) integrates a source (oscillator or synthesizer) with the VDI AMC. A VDI Mixer / Amplifier / Multiplier Chain (MixAMC) requires a customer low frequency local oscillator. A VDI Receiver (Rx) integrates the LO drive oscillator with the Mixer and LO Chain for turn-key operation.

Standard AMCs (SGXs) and standard MixAMCs (SAXs) have been developed to provide high performance RF drive multiplication and downconversion for full waveguide band coverage. These systems can be used to extend traditional

spectrum analyzers and signal generators into the THz and mm-wave ranges. VDI's SGXs and SAXs offer various modes of operation. VDI SGXs can be operated in standard frequency mode (<20GHz, 10dBm nominal) or high frequency RF drive mode (<45GHz, 0dBm nominal). VDI SAXs can also operate in standard and high frequency LO drive modes. Customers also have the option to operate SAXs for block-downconversion (<20GHz IF) or as a spectrum analyzer extender. SGXs and SAXs are available from WR15 (50-75GHz) to WM164 (1,100-1,500GHz).

VDI offers both narrow-band high-power and broadband low-power systems. High power systems use VDI's D-series X2 multipliers to achieve maximum multiplier efficiency and power handling. VDI has developed many high power systems for special customer applications, such as a novel multiplier based source with output power of >200mW at 263GHz.

Reconfigurable / modular AMCs are also available upon request.

Your Source For Terahertz and mm-Wave Products
Design and Manufacture of Millimeter Wave and Terahertz Devices, Components and Systems



Magnetische Resonanzspektroskopie

Magnetic Resonance Spectroscopy

www.gdch.de/nmr

Fachgruppe in der Gesellschaft Deutscher Chemiker
Division of the German Chemical Society

The Network for Magnetic Resonance Spectroscopists

Since its foundation in 1978, the **Magnetic Resonance Discussion Group** (FGMR) of the German Chemical Society (GDCh) aims to foster the technical and scientific advances in all disciplines of magnetic resonance spectroscopy, to represent the interests of the members and to communicate the importance of the method to the various branches of fundamental and applied science.

The group provides a platform and network for contacts between all scientists active in this very multidisciplinary research area at universities, in industry and at other scientific institutions in Germany and abroad. Also technicians and engineers are cordially welcome as members.

An open exchange of ideas, opinions, and experiences among scientists, experimentalists and theorists in chemistry, biology, physics, life sciences, medicine, food chemistry/technology, polymer and material sciences highlights the decisively interdisciplinary character of magnetic resonance methods and their applications.

More than 450 members are in permanent and intense communication to interchange ideas and experiences, especially fostered by the annual division meeting. Every second year this meeting is organized as a joint event with varying European magnetic resonance discussion groups to establish and intensify international contacts. Furthermore, the FGMR is in close contact with the European conference EUROMAR.

The NMR discussion group focuses on the support of young academics. This is mainly manifested by the annual **Ernst-Award**, dedicated to a maximum of three doctoral students as main authors of an outstanding publication in a renowned journal.

Since 2015, the **Felix-Bloch-Lecture** honors principal investigators for outstanding contributions to the progress of magnetic resonance spectroscopy.

Why join the Discussion Group?

- Supports your career by providing access to many professional contacts (networking)
- Easy contact to potential cooperation partners
- Annual meeting and continuing education Access to the GDCh network
- Reduced registration fees for scientific meetings

Especially for Students:

- Significantly reduced registration to the annual meeting
- Extra tutorials on the occasion of the annual meetings
- Reduced fee for numerous GDCh-offers and programs

How to Join the Group?

Members of the GDCh can apply for membership in the group. The annual fee is 10 € (students: 5 €).

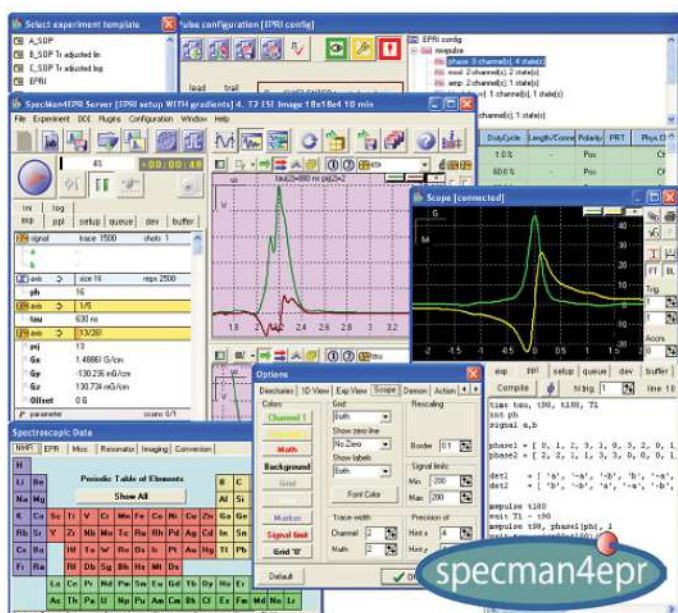
EPR is represented in a subdivision of the MR division and is connected as a working group to the European Federation of EPR groups.

SpecMan4EPR: Software for Pulse and CW EPR Instruments

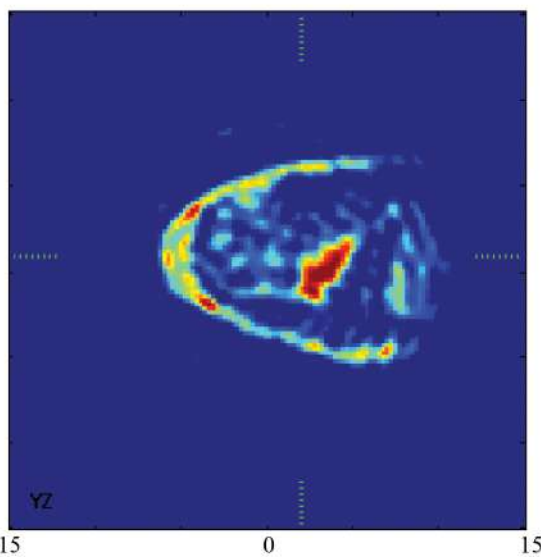
Connecting Spectrometers to People

Every EPR instrument requires a control software. While commercial products are supplied with a software, the designers of the unique solutions face the software programming challenge on their own. FeMi Instruments presents a solution to this problem.

- ◆ **SpecMan4EPR** is a versatile control and acquisition software for pulse and CW EPR instruments¹
- ◆ **Friendly** user support, adaptation of software for changing needs during the lifetime of the instrument
- ◆ **Unified** user experience for different instruments, rapid learning curve
- ◆ **Compatible** with the commonly used devices and interfaces
- ◆ **Expandable** to new devices, including custom-built ones
- ◆ **Numerous** applications from low frequency imagers to high field DNP instruments



Front-end windows and dialogs of the SpecMan4EPR



A 300 μm slice of 3D EPR image of tumor bearing mouse leg obtained using SpecMan4EPR. 250 MHz pulse imager.

- ◆ **Pulse Programming Language** adapted for pulse and arbitrary waveform generators;
- ◆ **Pulse shape library** and loadable pulse shapes;
- ◆ **Device-independent pulse programming language**; acquisition of multiple time traces during single pulse sequence;
- ◆ **Four-dimensional experiments**; linear, logarithmic or table-based definition of ANY device or experiment parameter;
- ◆ **In-scope Fourier transformation** and baseline correction; time-trace baseline subtraction.

Related products

- ◆ **Complete acquisition console** for EPR spectrometer;
- ◆ **PCB boards design** and manufacturing;
- ◆ **MATLAB data processing code**



<http://specman4epr.com/>
<http://femi.specman4epr.com/>



boris.epel@specman4epr.com

¹Epel B. *et al.*, Concepts in Magnetic Resonance, **26B**, 36 (2005)

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Future plans

- **Networking platform**
- **EPR database** (including software, lists of EPR groups, scripts from EPR schools & courses, seminal papers)
- **Extension of the support for young scientists** (with e.g. EPR schools, position posts)

Your ideas?
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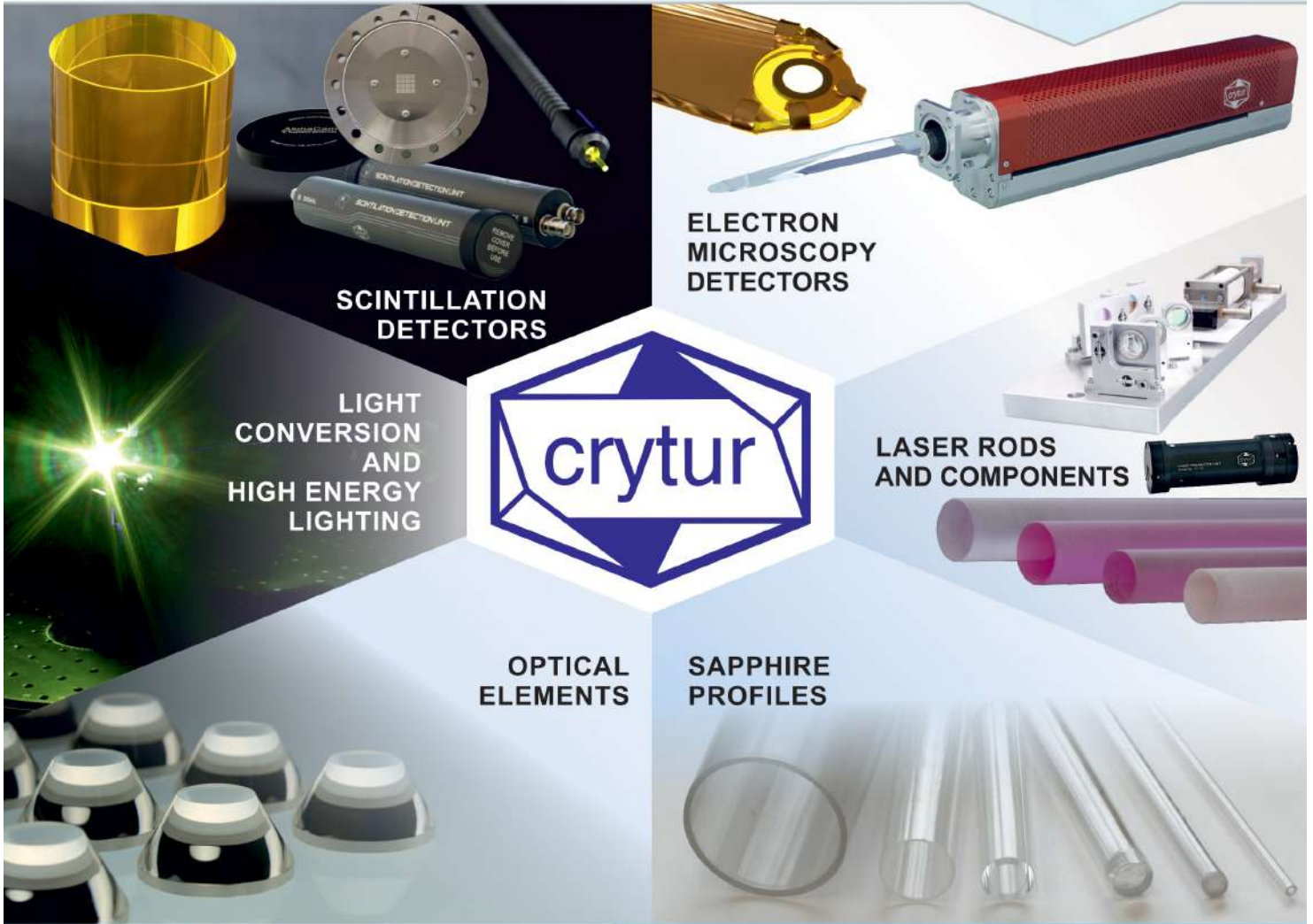
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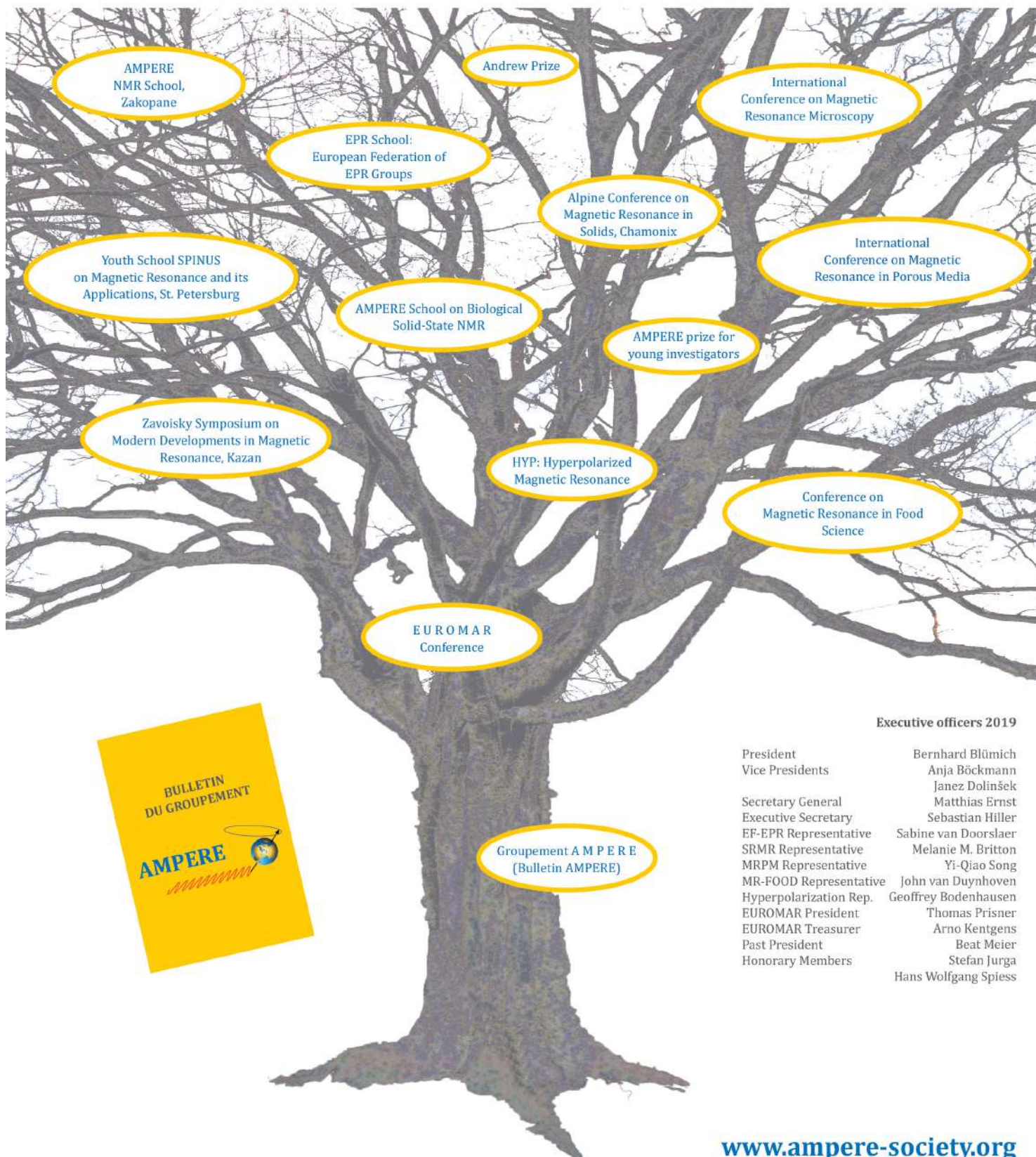
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The Groupement AMPERE (Atomes et Molécules Par Études Radio-ÉLECTRIQUES) is a European association of scientists with the mission to promote activities in magnetic resonance and related phenomena. It was founded in France in 1951 and was incorporated as a European organization in Switzerland in 1956.

Although the roots and the basic activities are in Europe, its members are from all over the world. Today it is the umbrella organization for several interest groups representing various aspects of magnetic resonance. The EUROMAR Conference is the annual general Conference of the AMPERE Society covering all fields of magnetic-resonance research.



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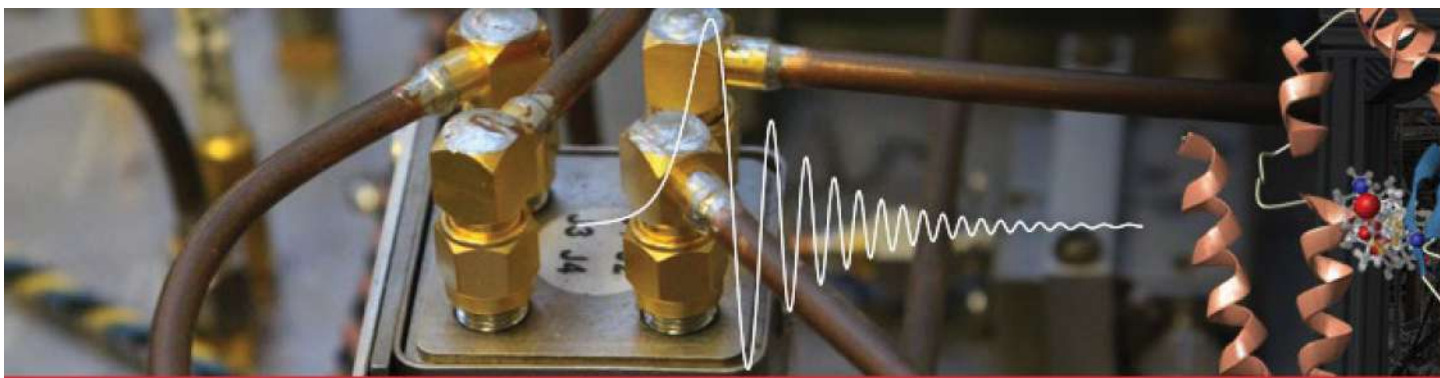
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SEM

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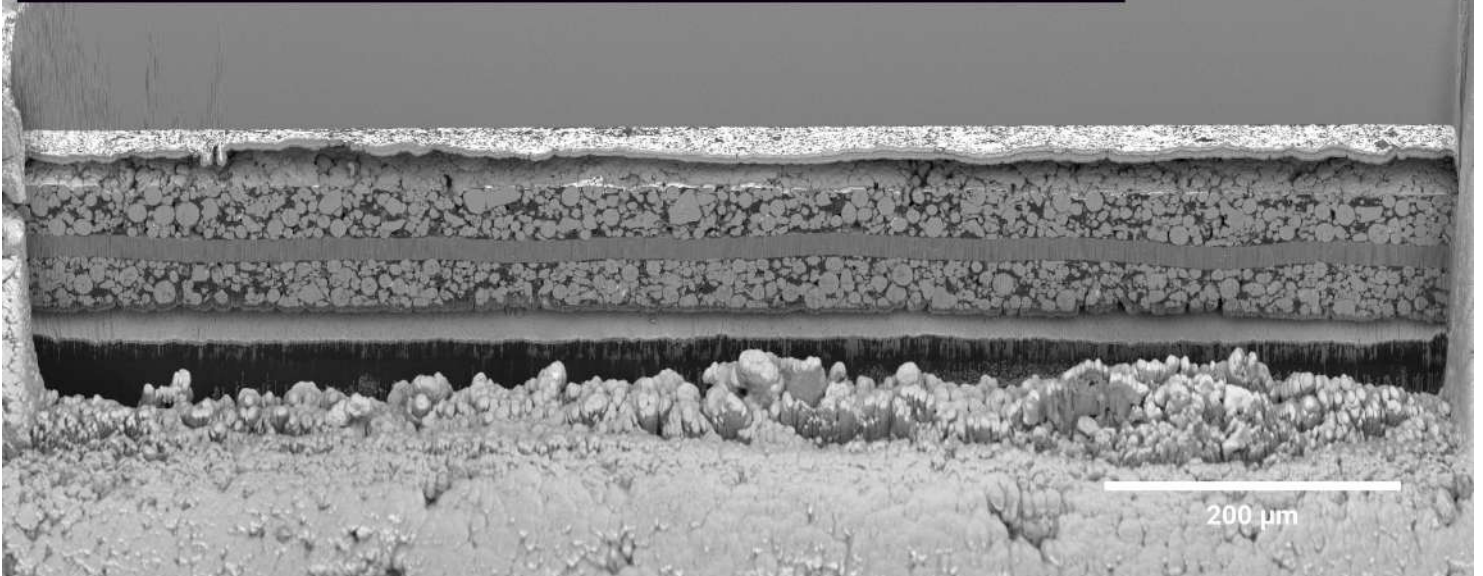
SharedEPR

The **SharedEPR** Network is an NSF funded initiative designed to bring together scientists from the fields of chemistry, biochemistry, physics, materials science, medicine, and biology with the goal of advancing the field of EPR spectroscopy. **Funding is available to support activities and events related to EPR.** Whether you are an experienced EPR researcher or new to the field, we invite you to become a participant in the Network, and join the community of EPR researchers! Visit our website for more information.

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6. PROGRAM

DAY 1 MONDAY 18TH NOVEMBER

18:30 – 21:30 Welcome Mixer

DAY 2 TUESDAY 19TH NOVEMBER

09:00 – 09:30 Welcome

**09:30 – 10:30 1. Fundamental Theory of EPR
Quantum Mechanics (Edgar Groenen)**

10:30 – 11:00 Coffee break

11:00 – 12:30 Student presentation

12:30 – 13:30 Lunch

13:30 – 15:30 Free time

**15:30 – 17:00 2. Relaxation processes
(Thomas Prisner)**

17:00 – 17:30 Coffee break

**17:30 – 19:00 2. Relaxation processes
(Thomas Prisner)**

19:00 – 20:00 Dinner

20:00 – Free evening

DAY 3 WEDNESDAY 20TH NOVEMBER

**09:00 – 10:30 4. Quantum chemical calculations,
ORCA tutorials (Frank Neese)**

10:30 – 11:00 Coffee break

**11:00 – 12:30 5. MW propagation - Quasi Optics
(Richard Wylde)**

12:30 – 13:30 Lunch

13:30 – 15:30 Free time

15:30 – 17:00 6. EasySpin (Stefan Stoll)

17:00 – 17:30 Coffee break

**17:30 – 19:00 7. MW technology – generation
(Jeffrey Hesler)**

19:00 – 20:00 Dinner

20:00 – 21:30 Poster Session I

DAY 4 THURSDAY 21ST NOVEMBER

**09:00 – 10:30 8. Introduction to NMR
(Lukáš Žídek)**

10:30 – 11:00 Coffee break

11:00 – 12:30 9. DNP, ENDOR (Marina Bennati)

12:30 – 13:30 Lunch

13:30 – 15:30 Free time

15:30 – 17:00 Free time / join activity

17:00 – 17:30 Coffee break

**17:30 – 19:00 Parallel tutorials session / class rooms:
MMM tutorials, EasySpin Tutorials,
Blackboard, DEER tutorials**

19:00 – 20:00 Dinner

20:00 – 21:30 Poster Session II

DAY 5 FRIDAY 22ND NOVEMBER

**09:00 – 10:30 11. ESEEM, HYSORE
(Sabine van Doorslaer)**

10:30 – 11:00 Coffee break

**11:00 – 12:30 12. ELDOR detected NMR
(Daniella Goldfarb)**

12:30 – 13:30 Lunch

13:30 – 15:30 Free time

15:30 – 17:00 Free time / join activity

17:00 – 17:30 Coffee break

17:30 – 19:00 Free time / join activity

19:00 – 20:00 Dinner

20:00 – Free evening

DAY 6 SATURDAY 23RD NOVEMBER

**09:00 – 10:30 13. Multi Frequency EPR and transition
metal complexes**

(Alexander Schnegg)

10:30 – 11:00 Coffee break

**11:00 – 12:30 14. Optically Detected Magnetic
Resonance (Jörg Wrachtrup)**

12:30 – 13:30 Lunch

13:30 – 15:30 Free time

15:30 – 17:00 15. Transient EPR (Serge Gambarelli)

17:00 – 17:30 Coffee break

**17:30 – 19:00 Parallel tutorials session / class rooms:
MMM tutorials, EasySpin Tutorials,**

Blackboard, DEER tutorials

19:00 – 20:00 Dinner

20:00 – Free evening

DAY 7 SUNDAY 24TH NOVEMBER

**09:00 – 10:30 16. Biological applications of EPR
(Marilena Di Valentin)**

10:30 – 11:00 Coffee break

11:00 – 12:30 17. EPR imaging (Boris Epel)

12:30 – 13:30 Lunch

13:30 – 15:30 Free time

**15:30 – 17:00 18. Materials, surfaces, powders
(Piotr Pietrzyk)**

17:00 – 17:30 Coffee break

17:30 – 19:00 Parallel tutorials session / class rooms:

MMM tutorials, EasySpin Tutorials,

Blackboard, DEER tutorials

19:00 – 19:30 Organizers word

19:30 – 20:00 Students Awards

20:00 – 21:30 Final Mixer

DAY 8 MONDAY 25TH NOVEMBER

09:00 – 10:30 19. Rapid Scan EPR (Mark Tseytlin)

10:30 – 11:00 Coffee break

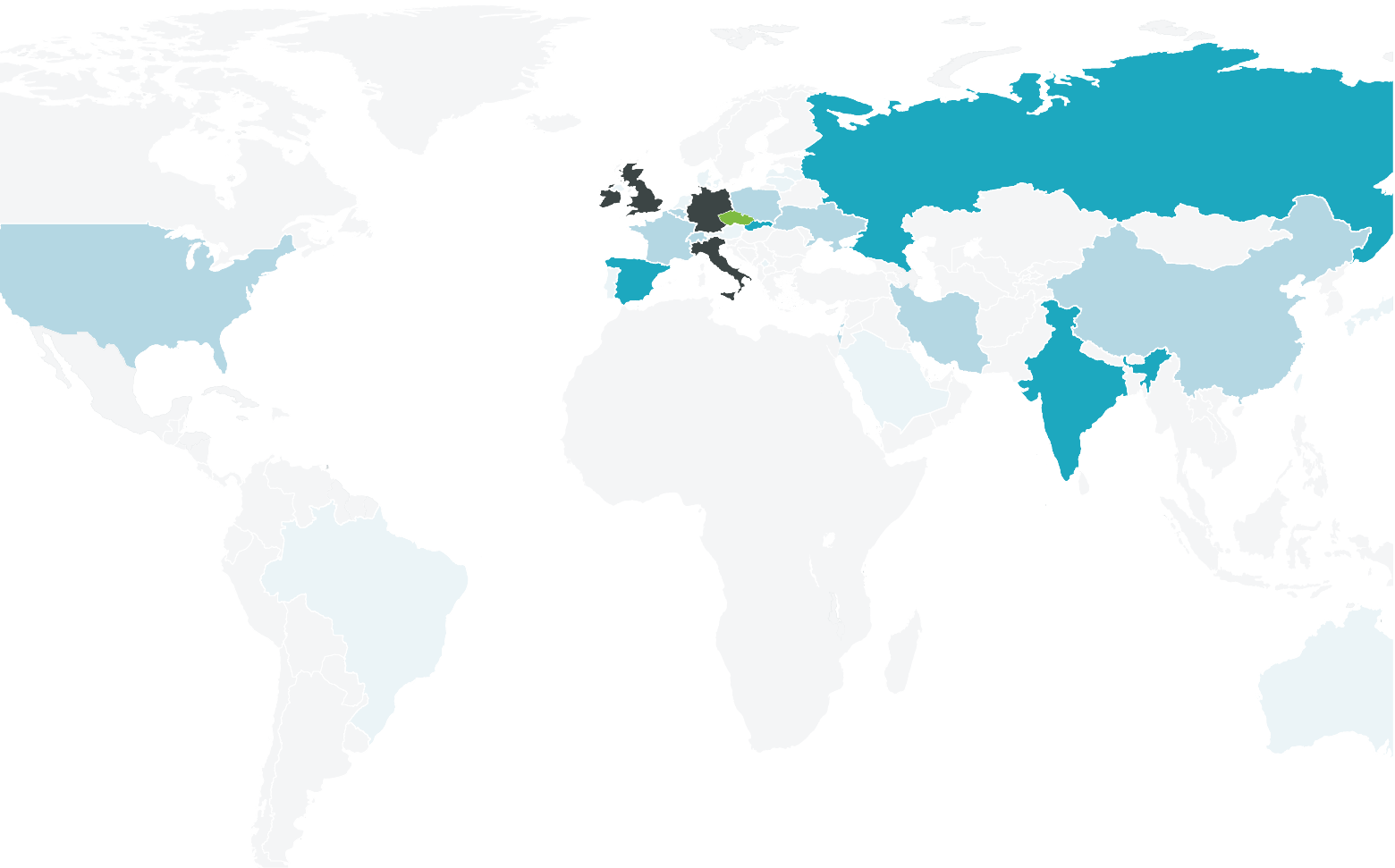
11:00 – 12:30 20. High Frequency EPR (Graham Smith)

12:30 – 13:30 Lunch

13:30 – 15:30 Free time

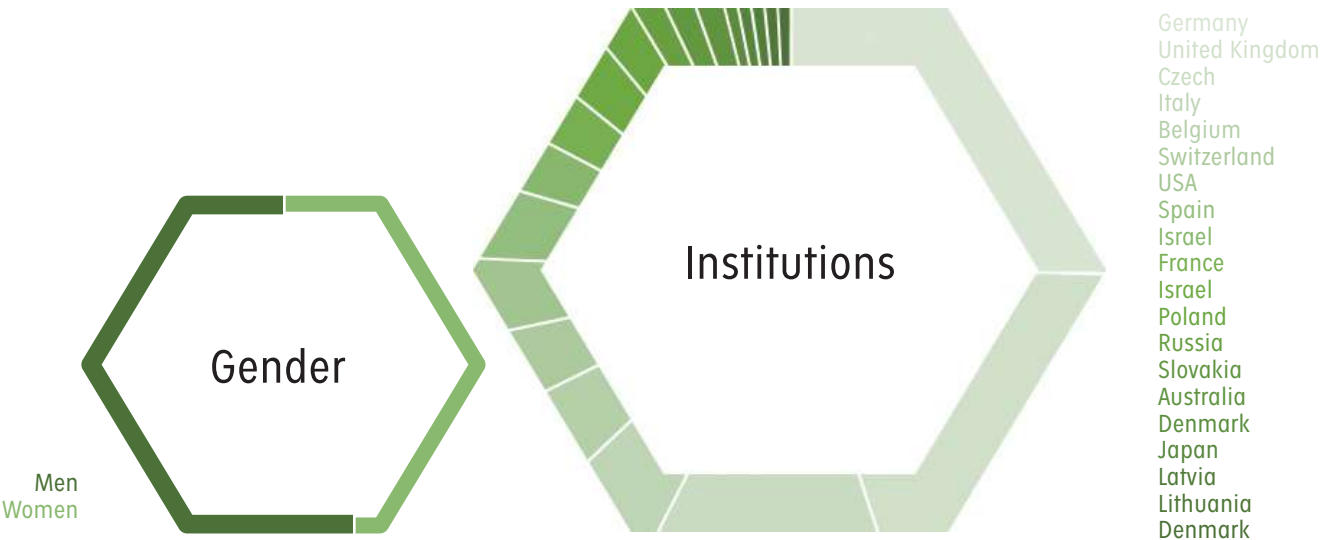
15:30 – 21:30 Departure

7. PARTICIPANTS



EFEPR Participants - Nationality

- > 15
- > 5
- > 1
- 1



PARTICIPANTS GROUP PHOTO



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8. POSTERS



From left: **Edgar Groenen**, POSTER WINNERS: Fabian Hecker, Francesco Torricella, Laura Esteban Hofer, Matthias Brettschneider, Tobias Hett, Marianne Le Dantec, **Petr Neugebauer**

1. **Katrin Ackermann**

Resolving the true distance distribution in homo-multimers

2. **Erika Aloj**

Spin-label EPR and spin-echoes in frozen phosphatidylcholine membranes: librational dynamics and solvent properties

3. **Seham Alzamanan**

Time-Resolved EPR of Ir(III) Photon Upconversion

4. **Lewis Martyn Antill**

Spatiotemporal measurement of cryptochromes for animal magnetoreception

5. **Andris Antuzevics**

EPR detection of Eu³⁺ ion distribution in glass ceramics

6. **Zdeněk Baďura**

Electron paramagnetic resonance as a powerful technique for identifying mechanism of hydrogen production with reduced TiO₂

7. **Zuzana Barbieriková**

Photoinduced processes on the semiconductor photocatalysts from the perspective of EPR spin trapping technique

8. **Euan Bassey**

Investigating high-voltage, high-capacity redox couples in sodium-ion battery cathodes

9. **Yasmin Ben-Ishay**

In-Cell Distance Measurements in Protein with Gd³⁺ Spin Labels

10. Arnau Bertran
Evolution of free radicals from novel Pt(IV) triazolato complexes following irradiation with visible light.
11. Jasleen Kaur Bindra
Spin Dynamics in Mn Doped ZnSe Quantum Dots
12. Maruan Alberto Bracci
Studying the role of proximal heme ligation in the reactivity of compound I by hyperfine spectroscopy
13. Matthias Bretschneider
Multiple quantum coherence EPR on nitroxide radicals
14. Adam Brookfield
EPSRC National EPR Facility.
15. Paolo Cleto Bruzzese
Activation of small molecules by cupric ions in MOFs and zeolites
16. Susanna Ciuti
Magnetophotoselection investigation on the triplet state of sulfonate porphyrins and their J-aggregates
17. Danhua Dai
An experimental access to the microwave saturation factor at 9.4 Tesla in liquid state
18. Marina Dajka
ESR investigation of the lipopolysaccharide transport (Lpt) system
19. Denisa Darvasiová
EPR/Uv-Vis-NIR spectroelectrochemistry of copper(II) complexes as potential anticancer drugs
20. Nir Dayan
Advanced surface resonators for electron spin resonance
21. Jessica Dröden
Investigation of intrinsically disordered proteins by spin-label EPR spectroscopy
22. Daria Dymnikova
Identification of Gd binding sites by EPR
23. Elena Edinach
Non-Kramers Tb³⁺ centers and evidence of their spin transfer to Ce³⁺ emitters in garnet crystals
24. Derek Elam
Application of Benchtop (X-band CW) EPR Spectroscopy in Chemical Industry
25. Christina Elsner
EPR Studies on the Apoptotic Bcl-2 Interactome
26. Asif Equbal
AWG-DNP Under Magic-Angle Spinning
27. Laura Esteban Hofer
Characterization of the role of the flexible linker of SRSF1 with EPR spectroscopy
28. Antonino Famulari
Towards tuning CYP450 reactivity: study of the oxidation cycle of CYP116B5 using H₂O₂
29. David Fioco
Advanced EPR study of Cr and Co paramagnetic metal centers in catalysis
30. Stuart Fisher
Conformational Changes in the Structure of Human Calmodulin in a Calcium-Peptide Dependant Manner.
31. Jörg Fischer
Gd(III)–Gd(III) Relaxation-Induced Dipolar Modulation Enhancement for In-Cell Electron Paramagnetic Resonance Distance Determination
32. Afonso Froes
Electron Paramagnetic Resonance Spectroscopy Studies of Metal Binding to the MamM C-Terminal Domain
33. Maximilian Gauger
Investigation of Mn²⁺ binding sites of a tetracycline aptamer using pulsed hyperfine-spectroscopy
34. Rugang Geng
Coherent Spin Manipulation in Organic Semiconductors
35. Ignacio Gimeno Alonso
Close-Up Analysis of Spin-Clock Transitions in Molecular Spin Qubits by On-Chip Broad-Band Spectroscopy
36. Laisvydas Giriūnas
EPR study of manganese-doped [(CH₃)₂NH₂][Cd(N₃)₃] metal-organic framework
37. Aathira Gopinath P
Protein folding and insertion by the BAM complex investigated using ESR spectroscopy
38. Andreas Gottscholl
Stimulated Microwave Emission from Optically Pumped Silicon Vacancy Defects in 4H Silicon Carbide for Maser Applications
39. Jeannine Grüne
Time-Resolved Optically Detected Magnetic Resonance of Spin-States involved in Thermally Activated Delayed Fluorescence
40. Andrea Guidetti
Mechanistic studies of photocatalysed thiyolation reaction of aryl-allyl species
41. Zainab Hafideddine
Development of globin-based biosensors: the immobilization of neuroglobin in mesoporous matrices
42. Fabian Hecker
170 High field ENDOR to investigate water-mediated PCET in E.coli ribonucleotide reductase
43. Melanie Heghmanns
Determination of redox potentials of plant-type ferredoxin isoforms via EPR spectroscopy
44. Shona Hepworth
Studying conformational dynamics of the SLC gene family homologues LeuT and VcINDY using advanced EPR techniques
45. Tobias Hett
Conformational Changes in a Cyclic Nucleotide-Binding Domain Studied by PELDOR Spectroscopy

46. Matthias Hoffmann

Protein P0 – the Protein that holds together Myelin at its inmost Folds

47. Jakub Hrubý

Graphene-Based Hybrid Material with Quantum Bits Prepared by Double Langmuir–Schaefer Method

48. David Hunger

Quinone-based single molecule magnets

49. Timothee Chauvire

In vivo pulse Electron Spin Resonance (ESR) characterization of Aerotaxis flavoprotein

50. Xiaoxun Chen

Pulsed photo-DNP to enhance the sensitivity of high-resolution magic-angle-spinning (MAS) NMR spectroscopy

51. Chandrima Jash

Exploring the Interaction of Calmodulin with its IQ target peptide by EPR distance measurements

52. Aneta Krasowska

Zinc(II) species in zeolite and their interaction with O₂ – generation of superoxo adducts in ZSM-5

53. Silvio Kunstner

Rapid scan EPR-on-a-chip

54. Valeria Lagostina

Functional Comparison of Quinone Reducing H⁺ Pumps

55. Oleksii Laguta

Multi-frequency rapid-scan EPR at millimetre wave frequencies

56. Tomáš Láznička

Design of mobile vacuum chamber for loading samples into High-Frequency Electron Paramagnetic Resonance spectrometer

57. Nolwenn Le Breton

EPR study of new metal complexes with bioinspired redox active ligands

58. Marianne Le Dantec

Electron Spin Resonance Spectroscopy of Rare-Earth-Ions at millikelvin temperatures

59. Florian Lehmann

Characterisation of binding and release of small molecules in serum albumin hydrogels

60. Yu-Kai Liao

EPR Investigations of Cr Species in Olefin Polymerization Heterogeneous Catalysts

61. Vega Lloveras Monserrat

Intramolecular Radicals Interaction in Polyradical Systems

62. Federico Lombardi

Topological spin-bearing defects in graphenoid molecules

63. Kwinten Maes

Multi-frequency EPR characterization of vanadium dopant sites in the metal-organic framework DUT-5(Al)

64. Giuseppina Magri

Perturbed Radicals in Catalysis: Detection of Reaction Inter-

mediates in Catalytic Reactions by Microwave Perturbed EPR Spectroscopy

65. Juraj Malinčík

Shape-persistent redox-active macrocycles.

66. Andriy Marko

Simulation of High Frequency Rapid Scan EPR Experiments

67. Gemma McGuire

The functional importance of Photosynthetic Complex I for photosynthetic energy balance

68. Shari Meichsner

Development of a Rigid Spin Label for Distance Measurements in Biomolecules via EPR

69. Jana Midlíková

Development of FTIR spectroscopy in high magnetic field

70. Andrea Maurizio Monti

Investigation on paramagnetic centres in quartz and their relation to the material's luminescence properties

71. Alvaro Montoya

Determining the Natural Binding Mode of Substrate in *Bacillus subtilis* Oxalate Decarboxylase by Pulsed EPR Spectroscopy

72. Bartosz Mozgawa

Generation of ROS on amorphous-crystalline composites via H₂O₂ decomposition

73. Fadis Murzakhanov

EPR study of synthetic calcium phosphate ceramics (tricalcium phosphate and hydroxyapatite) doped with manganese

74. David Nielsen

In-situ EPR on Cu-Zeolite catalysts for reduction of NO_x

75. Maria Oranges

Multi-frequency orientation selective copper(II)-nitroxide RIDME in model systems and proteins

76. Maria Papa

Unveiling the structure of RNA using EPR spectroscopy

77. Daniel Parker

EPR Spectroscopy of Single Molecules using Superconducting Microwave Resonators

78. Annalisa Pierro

Probing NarJ structural dynamics inside *E. coli* cells by EPR spectroscopy

79. Leonora Podvorica

EPR Characterization of Ti (III) Species in Heterogeneous Ziegler-Natta Catalysts

80. Ashley Redman

Triplet States of Donor-Acceptor Porphyrins

81. Laura Remmel

Biomolecular binding studies by EPR

82. Seyedeh Fardokht Rezayi

Application of Earth Abundant Metals (EAMs) for small molecule activation and C-C cross coupling

83. Katherine Richardson
Functional Comparison of Quinone Reducing H+ Pumps
84. Marcos Rubín Osanz
Development of superconducting lumped element resonators for molecular spin quantum processors
85. Michael Rudolph
Time-resolved PELDOR of the heterodimeric ABC exporter TmrAB
86. Hannah Russell
Measuring nanometre distance changes in biomolecules under pressure
87. Mohammad Samanipour
The non-innocent role of spintraps
88. Vinicius Tadeu Santana
Quantum phases in molecular materials
89. Takuma Sato
Defects investigation in BaSi₂ for solar cell applications
90. Manas Seal
Study of liquid-liquid phase separation of proteins by EPR spectroscopy
91. Ilenia Serra
Mechanistic insight in peroxidase activity towards industrial applications
92. Ekaterina Shabratova
EPR-on-a-Chip for Operando Experiments
93. Dennis Schäfter
Multi-Qubit Systems with Very Rigid Bridging Ligands
94. Niti Schindler
Investigation of multi-spin effects in pulse dipolar EPR spectroscopy using model systems
95. Florian Schöffmann
Binding characteristic of neuronal protein FA-transporter P2 characterized with spin-labeled fatty acids
96. Antoine Schuller
Unravelling the mechanism of Copper-mediated reactions using Electron Paramagnetic Resonance
97. Simon Lennard Schumann
EPR investigation of a tyrosine dyad in a ribonucleotide reductase-inspired model system
98. Kamila Sobańska
Electroprotic processes of the formation of reactive oxygen species on amorphous transition metal oxides surfaces
99. Antonín Sojka
Terahertz Magnetic Resonance Spectrometer for Electron Spin Dynamics Investigations
100. Artur Solodovnyk
Electrically Detected Magnetic Resonance setup based on a novel THz EPR Spectrometer
101. Jacob Spencer
Electron Paramagnetic Resonance (EPR) Study of Battery and Functional Materials
102. Anna Spitsyna
EPR study of human serum albumin using novel methanethiosulfonate derivative of OX063 Trityl
103. Luke St Marie
Spectroscopy of Single-Molecule Magnets Using Graphene Quantum Dots
104. Sonja Sternkopf
CW-EPR on organic light emitting diodes (OLEDs), polymers and pharmaceutical ingredients
105. Matúš Šedivý
Automated Alignment of a Quasi-Optical Table for a HFEPR Spectrometer
106. Tomáš Šolomek
Electron Hopping in Naphthalene-1,4:5,8-bis(dicarboximide) Chiral Covalent Organic Macrocycles
107. Rebekah Taylor
An EPR Investigation of the para-Xylene Oxidation Process
108. Michael Taylor
Shaped Pulses for Improving the Application of Electron Paramagnetic Resonance Spectroscopy for Studying Biomolecules
109. Kavipriya Thangavel
Elucidation of the Role of Paramagnetic Valence States of Highspin Transition Metals in MOF catalyst
110. Sonja Tischlik
Broadband shaped pulses for DEER spectroscopy
111. Francesco Torricella
PELDOR Investigation on Tilt Angles in Transmembrane b-Peptides
112. Niels Van Brempt
EPR spectroscopy on a selected set of structurally diverse globins from *Caenorhabditis elegans*
113. Agathe Vanas
Trityl Radicals for Distance Measurements: New Spin Labels and Pulsed Dipolar Spectroscopy in Narrow Lines
114. Maria Francesca Vicino
Conformational switching of the P2 hairpin from the guanine-II riboswitch
115. Nino Wili
Dressed electron spin resonance with phase-modulated pulses
116. Mario Winkler
The Static and Dynamic Electronic and Geometric Structure of Catalysts in Mesoporous Systems
117. Joshua Wort
Pulse EPR Shows Cu(II)-Chelates Label Double-Histidine Motifs More Efficiently with Lower Temperature
118. Yujie Zhao
High volume, high field, aqueous state EPR and DNP

Day 1, Monday

18:30 – 21:30	Welcome Mixer
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PROGRAMME

Day 2, Tuesday

09:00 – 09:30	Welcome
09:30 – 10:30	1. Fundamental Theory of EPR Quantum Mechanics (Eógar Groenen)
10:30 – 11:00	Coffee break
11:00 – 12:30	Student presentation
12:30 – 13:30	Lunch
13:30 – 15:30	Free time
15:30 – 17:00	2. Relaxation processes (Thomas Prisner)
17:00 – 17:30	Coffee break
17:30 – 19:00	3. EPR Instrumentation (Patrick Carl)
19:00 – 20:00	Dinner
20:00 –	Free evening/Activity

Day 3, Wednesday

4. Quantum chemical calculations, ORCA tutorials (Frank Neese)
Coffee break
5. MW propagation - Quasi Optics (Richard Wyde)
Lunch
Free time
6. EasySpin (Stefan Stoll)
Coffee break
7. MW technology – generation (Jeffrey Hesler)
Dinner
Poster Session I
Free evening/Activity

Day 4, Thursday

8. Introduction to NMR (Lukáš Židek)
Coffee break
9. DNP, ENDOR (Marina Bennati)
Lunch
Free time
10. Pulsed EPR, DEER (Gunnar Jeschke)
Coffee break
Parallel tutorials session / class rooms
Dinner
Poster Session II
Free evening/Activity

Day 5, Friday

11. ESEEM, HYSCORE (Sabine van Doorslaer)
Coffee break
12. ELDOR detected NMR (Daniella Goldfarb)
Lunch
VISIT OF BRNO Lab tours CEITEC BUT and CEITEC MU
Dinner
Free evening/Activity

Day 6, Saturday

13. Multi Frequency EPR and transition metal complexes (Alexander Schnegg)
Coffee break
14. Optically Detected Magnetic Resonance (Vadim Vorobyov)
Lunch
Free time
15. Transient EPR (Serge Gamberelli)
Coffee break
Parallel tutorials session / class rooms
Dinner
Free evening/Activity

Day 7, Sunday

16. Biological applications of EPR (Marilena Di Valentin)
Coffee break
17. EPR imaging (Boris Epel)
Lunch
Free time
18. Materials, surfaces, powders (Piotr Pietrzyk)
Coffee break
Parallel tutorials session / class rooms
Organizers word
Students Awards
Final Mixer

Day 8, Monday

09:00 – 10:30	19. Rapid Scan EPR (Mark Tseytlin)
10:30 – 11:00	Coffee break
11:00 – 12:30	20. High Frequency EPR (Graham Smith)
12:30 – 13:30	Lunch
13:30 – 15:30	Free time
15:30 – 21:30	Departure

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