



**MAGIC**

**2024**

**Frauenwörth  
Bayern**

Time		Monday	Tuesday	Wednesday	Thursday	Friday
8:00	8:45		breakfast / Klosterwirt			
9:00	9:05		<b>Welcome Musiksaal</b>	Fowler	Solà	Barquera
9:05	9:40		Bickelhaupt			
9:40	10:10		Monaco	Berger	Radenković	Olejniczac
10:10	10:40		Rončević	Stanger	Nasibullin	Dimitrova
10:40	11:00		coffee break			
11:00	11:40		Chauvin	Sundholm	Wu	Anstöter
11:40	12:05		Mallion	Poater	Cummings	Blasco
12:05	12:30		Dickens	Baranac-Stojanović	Đorđević	Puchta
12:30	14:00		check-in reception	free break	free break	free break
14:00	14:30	Helgaker		cultural prog. 2	Komorovsky	
14:30	15:10	Summa			Orozco	
15:10	15:35	Vanden Berghe			Mahmood	
15:35	16:00	coffee break			coffee break	
16:00	16:20	Ortmann			Malkin O.	
16:20	17:00	Malkin			Åström	
17:00	17:25	Havenith		Lehtola		
17:25	17:50	dinner / Klosterwirt		Djukić		
18:00	19:00	cultural prog. 1 + posters			conf. Dinner Schloßwirt	
19:00	21:00					
21:00	21:30					

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## Organizing committee

Raphael Berger    Guglielmo Monaco

# Timetable

SC: Session Chair, IT: Invited Talk.

## Tuesday, 10 of September

08:00–08:55	Breakfast // Klosterwirt		
09:00–09:05	Welcome remarks // Musiksaal		
09:05–09:40	SC	<b>Matthias Bickelhaupt</b> Amsterdam, Netherlands	Aromaticity: MO Picture of an Intuitive Concept
09:40–10:10	IT	<b>Guglielmo Monaco</b> Salerno, Italia	Recent Computational Tools for Magnetic Aromaticity
10:10–10:40	IT	<b>Igor Rončević</b> Oxford, United Kingdom	Aromaticity Reversals in Molecules and Materials
10:40–11:00	Coffee		
11:00–11:40	SC	<b>Remi Chauvin</b> Toulouse, France	Aromaticity, simple interpretations of a complex notion: from graph spectra to intrinsic ring currents
11:40–12:05	IT	<b>Roger Mallion</b> Canterbury, United Kingdom	tba
12:05–12:30	IT	<b>Timothy Dickens</b> Cambridge, United Kingdom	Clar's Goblet
12:30–14:30	Free Break		
14:30–15:10	SC	<b>Trygve Helgaker</b> Oslo, Norway	Molecular Dynamics and Rovibrational Spectra in a Magnetic Field
15:10–15:35	IT	<b>Francesco Summa</b> Salerno, Italy	From Current Density Tensor to Optical Rotation Power Density
15:35–16:00	IT	<b>Emiel Vanden Berghe</b> Ghent, Belgium	Navigating spin-transitions in magnetic fields by variationally tuning restored broken symmetries
16:00–16:20	Coffee		
16:20–17:00	SC	<b>Frank Ortmann</b> München, Germany	Understanding the electronic pi-system of 2D covalent organic frameworks with Wannier functions
17:00–17:25	IT	<b>Vladimir Malkin</b> Bratislava, Slovakia	Transmission of spin-polarisation by pi-orbitals
17:25–17:50	IT	<b>Remco Havenith</b> Groningen, Netherlands	Induced current densities in spin-crossover complexes
18:00–19:00	Dinner // Klosterwirt		
19:00–21:00	Bavarian Beers: History, Manufacturing and Tasting // Musiksaal		

## Wednesday, 11 of September

08:00-08:55	Breakfast // Klosterwirt		
09:00-09:40	SC	<b>Patrick Fowler</b> Sheffield, United Kingdom	Current-density mapping
09:40-10:10	IT	<b>Raphael Berger</b> Salzburg, Austria	Towards an Automated Qualitative and Quantitative Analyses of $J^B$
10:10-10:40	IT	<b>Amnon Stanger</b> Haifa, Israel	Aromaticity in Si and Ge three-membered rings
10:40-11:00	Coffee		
11:00-11:40	SC	<b>Dage Sundholm</b> Helsinki, Finland	Magnetically Induced Current-Density Susceptibilities in Porphyrinoids
11:40-12:05	IT	<b>Jordi Poater</b> Barcelona, Spain	New hybrid conjugation via boron cage extension
12:05-12:30	IT	<b>Marija Baranac-Stojanović</b> Belgrade, Serbia	The effect of BN substitution on aromaticity and HOMO-LUMO energy gap of coronene
12:30-14:00	Free Break		
14:00-17:50	Guided Tour Schloß Herrenchiemsee & German Constitution Convention		
18:00-19:00	Dinner // Klosterwirt		

## Thursday, 12 of September

08:00–08:55	Breakfast // Klosterwirt		
09:05–09:40	SC	<b>Miquel Solá</b> Girona, Spain	Challenging Conventions: Investigating the Limits of Diatropic and Paratropic Currents
09:40–10:10	IT	<b>Slavko Radenković</b> Kragujevac, Serbia	Calculation of current densities of large molecules
10:10–10:40	IT	<b>Rinat Nasibullin</b> Helsinki, Finland	Orbital contribution to magnetically induced ring currents
10:40–11:00	Coffee		
11:00–11:40	SC	<b>Judy Wu</b> Houston, USA	Antiaromaticity concepts and matching H-NMR to computed chemical shifts
11:40–12:05	IT	<b>Edward Cummings</b> York, United Kingdom	Annulene Aromaticity: Vertical vs Adiabatic Excitations and De-excitations
12:05–12:30	IT	<b>Sladana Đjordžević</b> Kragujevac, Serbia	Aromaticity in benzo-annelated perylenes
12:30–14:30	Free Break		
14:30–15:10	SC	<b>Stanislav Komorovsky</b> Bratislava, Slovakia	Current densities as a tool for analysis of magnetic properties in the relativistic domain
15:10–15:35	IT	<b>Mesias Orozco Ic</b> Helsinki, Finland	Core-electron contributions to the magnetic response of molecules with heavy elements
15:35–16:00	IT	<b>Atif Mahmood</b> Helsinki, Finland	The Pseudo- $\pi$ method and the current densities of porphyrinoid nanostructures
16:00–16:20	Coffee		
16:20–17:00	SC	<b>Olga Malkin</b> Bratislava, Slovakia	Solvent effects on $J$ -couplings
17:00–17:25	IT	<b>Hugo Åström</b> Helsinki, Finland	Insight on Gaussian basis set truncation errors in magnetic fields
17:25–17:50	IT	<b>Susi Lehtola</b> Helsinki, Finland	A call to arms: making the case for more reusable libraries
17:50–18:10	IT	<b>Nikolas Djukić</b> Regensburg, Germany	BAYHOST
19:00–21:30	Conference Dinner // Herreninsel		

## Friday, 13 of September

08:00–08:55	Breakfast // Klosterwirt		
09:00–09:40	SC	<b>José Berquera</b> Mexico City, Mexico	Similarities and differences of trace of the curl of the current density and the laplacian of the electron density topology
09:40–10:10	IT	<b>Małgorzata Olejniczak</b> Lille, France	On designing scalar descriptors of the magnetically-induced current density in molecular systems
10:10–10:40	IT	<b>Maria Dimitrova</b> Helsinki, Finland	Magnetic properties calculated using the Ampère-Maxwell
10:40–11:00	Coffee		
11:00–11:40	SC	<b>Cate Anstöter</b> Edinburgh, Scotland	Exploring the redox chemistry of BN-doped macrocycles
11:40–12:05	IT	<b>Daniel Blasco</b> Rioja, Spain	The aromatic nature of auracycles and diauracycles based on calculated ring-current strengths
12:05–12:30	IT	<b>Ralph Puchta</b> Erlangen, Germany	Hal(l)o Heterocycles
12:30	Closing and Departure		



## **Toroidal-Poloidal Decomposition of Magnetically-Induced Current Densities**

James R. Asher, *Slovak Academy of Sciences, Bratislava*

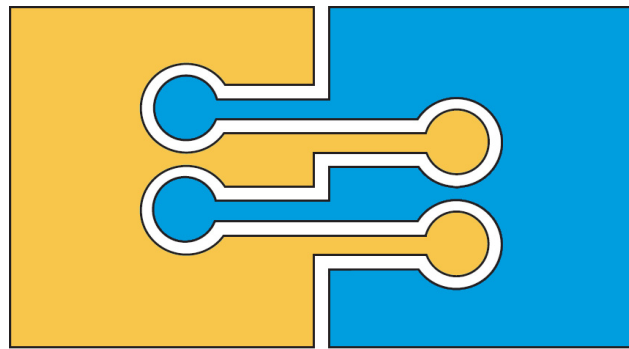
# List of Participants

Amnon Stanger	Technion-Israel Institute of Technology
Atif Mahmood	University of Helsinki
Cate Anstöter	University of Edinburgh
Dage Sundholm	University of Helsinki
Daniel Blasco Santana	University of Rioja
Edward Cummings	University of York
Emiel Vanden Berghe	University of Ghent
Francesco Summa	Università di Salerno
Frank Ortmann	Technical University Munich
Gosia Olejniczac	University of Warsaw
Guglielmo Monaco	Università di Salerno
Helgaker Trygve	University of Oslo
Henrik Ottosson	Uppsala University
Hugo Åström	University of Helsinki
Igor Roncevic	University of Oxford
James Asher	Slovak Academy of Sciences
Jordi Poater	University of Barcelona
José Barquera	Universidad Nacional Autonoma de México
Judy Wu	University of Houston
Maria Dimitrova	University of Helsinki
Marija Baranac-Stojanović	University of Belgrade
Matthias Bickelhaupt	University of Amsterdam
Mesias Orozco Ic	Donostia International Physics Center
Miquel Solà	University Girona
Olga Malkina	Slovak Academy of Sciences
Patrick Fowler	University of Sheffield
Ralph Puchta	University of Erlangen
Raphael Berger	University of Salzburg
Remco Havenith	University of Groningen
Remi Chauvin	University Toulouse III
Hline Rinat Nasibullin	University of Helsinki
Roger Mallion	Kent's College
Sladana Đjordžević	University of Kragujevac
Slavko Djukić	University of Regensburg
Slavko Radenkovic	University of Kragujevac
Stano Komorovsky	Slovak Academy of Sciences
Stefan Taubert	University of Helsinki
Susi Lehtola	University of Helsinki
Timothy Dickens	University of Cambridge
Vladimir Malkin	Slovak Academy of Sciences

# Partner Institutions and Sponsors

The conference is supported by the Paris-Lodron University of Salzburg, Austria.

## Cooperational Partners



B A Y H O S T

# Map



- A: Main pier
- B: Entry to the monastery
- C: Klosterwirt (breakfast and regular dinner place)
- D: accomodation area
- E: Musiksaal in the second floor
- F: little grocers shop
- G: Gasthaus zur Linde
- H: Inselwirt
- I: Inselbräu
- J: Beer garden
- K: fresh smoked local fish shops
- L: good place for a refreshing dip
- M: impressive old linden trees
- N: Nordsteg (alternative boat connection)

