

AROMATICITY 2025

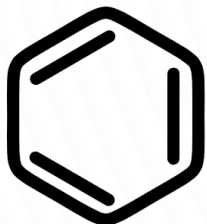
MERIDA, MEXICO, JANUARY 27-30, 2025

PROGRAM

VENUE: SALA MAYAMAX IN THE MAYAN WORLD MUSEUM OF MERIDA

MONDAY 27th

08:00 - 09:00	REGISTRATION
09:00 - 09:30	INAUGURATION
	<i>Chair Gabriel Merino</i>
09:30 - 10:00	Mesías Orozco-Ic, Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca, México Core-electron contributions to the magnetic response of molecules with heavy elements
10:00 - 10:30	Bo Durbeej, Linköping University, Sweden Improving the harmonic oscillator model of aromaticity with antiaromatic reference molecules
10:30 - 11:00	Hiroshi Shinokubo, Nagoya University, Japan Close π -stacking of antiaromatic porphyrins through four-electron multicentered bonding
11:00 - 11:30	COFFEE BREAK
	<i>Chair Thomas Heine</i>
11:30 - 12:00	Masaichi Saito, Saitama University, Japan Creation of σ -delocalization systems and their charge transport properties
12:00 - 12:30	Mercedes Alonso, Vrije Universiteit Brussel, Belgium Fine-tuning excited states using aromaticity
12:30 - 13:00	Gernot Frenking, Philipps-Universität Marburg, Germany How to stabilize antiaromatic compounds?
13:00 - 13:30	Francesc Teixidor, Institute of Materials Science of Barcelona, Spain The journey from the Hückel's $4n+2$ rule to the Wade's $2n+2$ rule
13:30 - 13:45	Sílvia Escayola, University of Stuttgart, Germany Navigating the challenges in designing double aromatic 2D and 3D molecules
13:45 - 14:00	Fernando Buendía-Zamudio, National University of Singapore, Singapore Formation of quasi-planar boron clusters applying topological path to smaller boron clusters
14:00 - 16:00	LUNCH
	<i>Chair Miquel Solà</i>
16:00 - 16:30	Fernando Cossío, Universidad del País Vasco, Spain/ Donostia International Physics Center, Spain Novel studies on the aromaticity of fused azaheterocycles and transition structures
16:30 - 17:00	Yoshimitsu Itoh, University of Tokyo, Japan Photo-responsive $[4n]$ annulene derivatives for functional polymers
17:00 - 17:30	Paul McGonigal, University of York, UK Breaking tropylium rings in the ground and excited states
17:30 - 18:00	Malika Jeffries-EL, Boston University, USA Design and synthesis of organic electronic materials
18:00 - 18:30	Juan Casado, Universidad de Málaga, Spain Topological structure of polyconjugated molecules and the design of open-shell systems



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18:30 – 20:00

WELCOME RECEPTION

TUESDAY 28th

Chair | Fernando Cossío

9:00 – 9:30

Jordi Poater, Universitat de Barcelona, Spain

Non-classical boron cluster-phosphonium conjugates and other boron cage extensions

9:30 – 10:00

José Enrique Barquera-Lozada, Universidad Nacional Autónoma de México, México

Global and local electron delocalization in covalent organic frameworks (COFs)

10:00 – 10:30

Norihito Tokitoh, Kyoto University, Japan

New insights in the chemistry of heavier aryl anions

10:30 – 11:00

Marija Baranac-Stojanović, University of Belgrade, Serbia

(Anti)aromaticity of cyclo[n]carbons ($n = 6 - 24$)

11:00 – 11:30

COFFEE BREAK

Chair | Renana Gershoni-Poranne

11:30 – 12:00

Yosadara Ruiz-Morales, Instituto Mexicano del Petróleo, México

Y-Rule aromaticity and Y-rule mapping in oil asphaltenes. Implications in the oil industry

12:00 – 12:30

Judy Wu, University of Houston, USA

Finding ways to cheat transition state theory (better) in chemical reactions

12:30 – 13:00

Israel Fernández, Universidad Complutense de Madrid, Spain

Transition state aromaticity and its relationship with chemical reactivity

13:00 – 13:30

Aurelio Mateo-Alonso, University of the Basque Country, Spain

Molecular graphene nanoribbons

13:30 – 13:45

Théo P. Gonçalves, King Abdullah University of Science and Technology, Saudi Arabia

Aromaticity-active ligands in catalysis

13:45 – 14:00

Ricardo Pino-Rios, Universidad Arturo Prat, Chile

The Glidewell-Lloyd rule: recent advances and applications

14:00-16:00

LUNCH

Chair | Mercedes Alonso

16:00 – 16:30

Alvaro Muñoz, Universidad San Sebastián, Chile

Multiple aromatic units within a single molecular structure. Overall aromaticity in local aromatic aggregates.

16:30 – 17:00

Irena Stara, Czech Academy of Sciences, Czech Republic

Helicenes as attractive building blocks for complex chiral nanocarbons

17:00 – 17:30

Renana Gershoni-Poranne, Israel Institute of Technology, Israel

Mission imPASSible: deep learning decodes aromatic systems

17:30 – 18:00

Henrik Ottosson, Uppsala University, Sweden

Deciphering the astrophotochemical inertness of H_3^+ at the molecular level

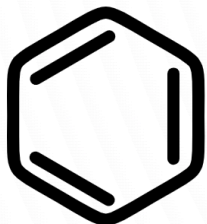
18:00 – 18:30

Ivan A Popov, Washington State University, USA

Localization vs. delocalization: Geometric and electronic structure evolution of group 13 hydrides

18:30 – 20:00

POSTER SESSION

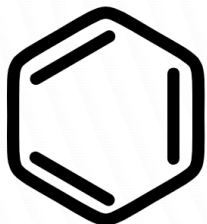


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WEDNESDAY 29th

- Chair | Yosadara Ruiz-Morales*
- 9:00 – 9:30 Igor Alabugin, Florida State University, USA
Cyclizations and cycloaromatizations: interplay between aromaticity and antiaromaticity
- 9:30 – 10:00 Masaaki Nakamoto, Hiroshima University, Japan
A stable silapyramidane from silyl cyclobutadiene and a single silicon atom
- 10:00 – 10:30 Guglielmo Monaco, Università di Salerno, Italy
Advancements in the calculation of the magnetic response and applications in the realm of magnetic aromaticity
- 10:30 – 11:00 Thomas Heine, School of Science, TU Dresden, Dresden, Germany
Magnetic carbon
- 11:00 – 11:30 **COFFEE BREAK**
- Chair | Jordi Poater*
- 11:30 – 12:00 Ryohei Kishi, Osaka University, Japan
On the relationship between stacked-ring aromaticity and Baird's rule
- 12:00 – 12:30 Clara Viñas, Institute of Materials Science of Barcelona, Spain
Revolutionizing (bio)materials: the experimental breakthrough of 3d aromaticity
- 12:30 – 13:00 John D. Tovar, Johns Hopkins University, USA
Unusual conjugation topologies and their impact on delocalization within pi-electron materials
- 13:00 – 13:30 Igor Rončević, University of Oxford, UK
Anti-aromaticity and electronic structure: from cyclocarbons to 2D materials
- 13:30 – 14:00 Said Jalife Jacobo, University of Houston, USA
Modulating paratropicity in polycyclic antiaromatic hydrocarbons
- 14:00 – 16:00 **LUNCH**
- Chair | Judy Wu*
- 16:00 – 16:30 Diego Peña, Universidade de Santiago de Compostela, Spain
Challenges and opportunities in the on-surface synthesis of carbon-based aromatic nanostructures
- 16:30 – 17:00 Aiko Fukazawa, Kyoto University, Japan
Synthesis, antiaromatic character, and coordination behavior of highly antiaromatic thiophene-fused pentalenes
- 17:00 – 18:00 Henrik Ottosson, Uppsala University, Sweden
Round table

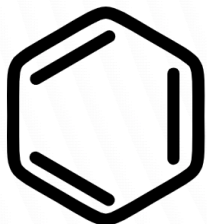


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THURSDAY 30th

9:00 – 13:00	FREE MORNING. VISIT TO UXMAL <i>Chair Henrik Ottosson</i>
13:00 -13:30	Amnon Stanger, Technion – Israel Institute of Technology, Israel Aroma 2.0
13:30 – 14:00	Miquel Solà, University of Girona, Spain The aromaticity and the relative stability of the n,π^* states of heteroaromatic compounds
14:00 – 14:30	Dage Sundholm, University of Helsinki, Finland Calculating orbital contributions to the magnetically induced current density using gauge-including atomic orbitals
14:30 – 15:00	Eduard Matito, Donostia International Physics Centre, Spain/ Ikerbasque Foundation, Spain Efficient assessment of aromaticity through electron-delocalization metrics
15:00 – 16:00	Henrik Ottosson, Uppsala University, Sweden Round table
18:00	CLOSING DINNER



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Gabriel Merino (Cinvestav Mérida)

Miquel Solà (Universitat de Girona)

Henrik Ottosson (Uppsala Universitet)

Local Organizing Committee

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Elier E. Abreu-Martínez

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