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**
	*Chair	Gabriel Merino*
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**
	*Chair	Thomas Heine*
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**
	*Chair	Miquel Solà*
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

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	Norihiro 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**

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

THURSDAY 30th

9:00 – 13:00	**FREE MORNING. VISIT TO UXMAL**
	Chair | Henrik Ottosson
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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Organizers

Gabriel Merino (Cinvestav Mérida)
Miquel Solà (Universitat de Girona)
Henrik Ottosson (Uppsala Universitet)

Local Organizing Committee

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