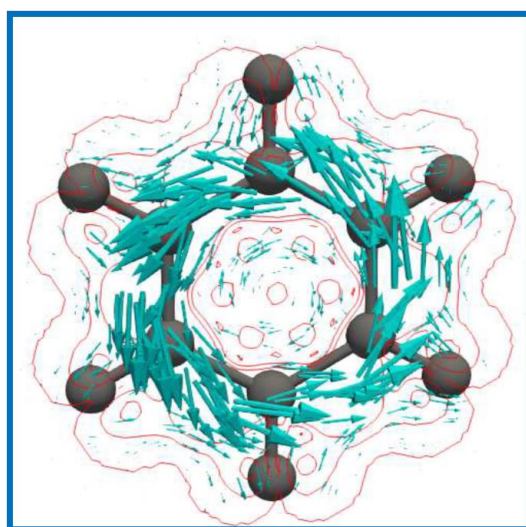


MAGIC – 2018

3rd workshop of **M**AGnetically **I**nduced **C**urrents in molecules



PROGRAM

23 – 28 September 2018, Kragujevac
Serbia

Sunday (23.09)	
	<u>Hotel Kragujevac</u> ARRIVAL AND REGISTRATION
19:30 - 22:00	WELCOME DINNER: Restaurant <i>Koš</i>, Kragujevac

Monday (24.09)	
07:30 - 09:00	Breakfast
09:00 - 09:20	OPENING CEREMONY
09:30 - 10:15	P. Lazzeretti Gauge invariance and origin independence of electronic charge density and current density induced by optical fields
10:15 - 10:45	Coffee break
10:45 - 11:30	R. Mallion Topological Ring-Currents and Clar Sextets in Fully Benzenoid Hydrocarbons
11:30 - 12:05	T. Dickens Topological Ring-Currents and Bond-Currents in Some Neutral and Dianionic Altans of Corannulene and Coronene
12:05 - 12:20	Discussion
13:00 - 14:00	Lunch
14:00 - 14:45	H. Ottosson On Triplet State Baird (Anti)Aromaticity in Polycyclic, Macrocyclic and Through-Space Conjugated Hydrocarbons
14:45 - 15:20	O. Malkina A mystery of a through-space indirect NMR spin-spin coupling
15:20 - 15:50	Coffee break
15:50 - 16:25	M. Baranac-Stojanović Are Substituent Resonance Effects Responsible for Variations of ¹ H NMR Chemical Shifts in Aniline and Nitrobenzene?
17:00 - 19:00	The Memorial Park October in Kragujevac
19:00 - 23:00	DINNER: Restaurant <i>Oranica</i>, Kragujevac

Tuesday (25.09)	
07:30 - 09:00	Breakfast
09:00 - 09:45	D. Sundholm The Gauge-Including Magnetically Induced Currents Method
09:45 - 10:20	I. Benkyi Magnetically Induced Current Densities in Porphycene and Porphycene Isomers
10:20 - 10:50	Coffee break
10:50 - 11:25	L. Wirz Magnetically induced ring-current strengths in twisted annulenes
11:25 - 12:00	V. Liegeois Investigation of Magnetically Induced Current Density on Helicene compounds
12:00 - 12:15	Discussion
13:00 - 14:00	Lunch
14:00 - 14:45	P. Karadakov What is the Multiplicity of the Bonds in C ₂ and S ₂ N ₂ and Can We Say that S ₂ N ₂ is Aromatic?
14:45 - 15:20	R. Puchta Nucleus Independent Chemistry by Schleyer
15:20 - 15:50	Coffee break
15:50 - 16:25	J. Poater Link between aromatic polycyclic aromatic hydrocarbons and boron hydrides
16:25 - 17:00	S. Radenković Double aromaticity and ring currents in triple-layered beryllium-boron clusters
17:15 - 19:00	Guided City Tour
19:30 - 23:00	DINNER: Restaurant <i>Panorama</i> (Hotel Kragujevac)

Wednesday (26.09)	
07:30 - 09:00	Breakfast
09:00 - 09:45	T. Helgaker Closed-Shell Molecular Paramagnetism
09:45 - 10:30	R. Berger A connection between Jahn-Teller distortion and paratropic currents by symmetry
10:30 - 11:00	Coffee break
11:00 - 11:35	A. Teale Magnetically Induced Currents in Strong Fields
11:35 - 12:10	M. Dimitrova Halomethanes and CH fragments in strong magnetic fields
12:10 - 12:25	Discussion
13:00 - 14:00	Lunch
14:30 - 19:00	EXCURSION: Oplenac, Topola
19:00 - 23:00	DINNER: Winery Aleksandrović, Topola

Thursday (27.09)	
07:30 - 09:00	Breakfast
09:00 - 09:45	G. Monaco AACID: the Anisotropy of the Asymmetric magnetically Induced Current Density tensor
09:45 - 10:20	A. Berger Gauge-invariant magnetic response properties from the induced current
10:20 - 10:50	Coffee break
10:50 - 11:25	S. Sen A local tensor that unifies kinetic energy density and vorticity dependent exchange-correlation functionals
11:25 - 12:00	M. Olejniczak Magnetic properties in the Frozen Density Embedding framework – lessons from the topological data analysis perspective
12:00 - 12:15	Discussion
13:00 - 14:00	Lunch
14:00 - 14:45	H. Fliegl Theoretical studies of magnetically induced currents as a tool for understanding the aromatic character of novel compounds
14:45 - 15:20	M. Repisky Visualization of current densities calculated by means of the relativistic two- and four-component electron dynamics
15:20 - 15:50	Coffee break
15:50 - 16:25	J. Asher An Animated Visualisation of Orbital Angular Momentum and Spin-Orbit Coupling
16:25 - 17:00	V. Malkin Visualization of EPR Hyperfine Structure Coupling Pathways
17:00 - 17:15	Discussion
17:05 - 19:00	Free time
19:00 - 21:00	DINNER: Hotel Kragujevac

Friday (28.09)	
07:30 - 09:00	Breakfast
09:00 - 09:35	J. Đurđević Nikolić Local aromaticity in phosphorus and nitrogen analogues of acenaphthylenes
09:35 - 10:10	B. Furtula Methods for partitioning the π -electrons by rings in polycyclic aromatic hydrocarbons as parameters for the qualitative elucidation of ring currents
10:10 - 10:40	Coffee break
10:40 - 11:40	Discussion
11:40 - 12:10	Free time
13:00 - 14:00	Lunch
	Departure