

Thursday – September 12th

III WBTC – Workshop on Bioinorganic Theoretical Chemistry – (Room 1B – Main Floor)

13:00 – 13:30	Reception - Registration
13:30 – 13:40	Workshop Opening <i>Chair: Luiz Antônio Sodr� Costa</i>
13:40 – 14:30	Lecture 1: Paula Homem-de-Melo (UFABC) <i>“Organometallic compounds do not use Jacob’s Ladder”</i>
14:30 – 15:20	Lecture 2: J�lio C. S. da Silva (UFAL) <i>“Elucidating pMMO Mechanisms: Computational Strategies for Bioinorganic Challenges”</i>
15:20 – 15:40	Coffee Break
15:40 – 16:30	Lecture 3: Sylvio Canuto (USP) <i>“Combined QM/MM studies of Molecular Spectroscopy in Different Environments from Simple Homogeneous Liquids to Proteins”</i>
16:30 – 17:20	Lecture 4: John Mack (Rhodes University, South Africa) <i>“The rational design of porphyrin and BODIPY analogues for biomedical and nonlinear optical applications”</i>
17:20 – 17:30	Closing Session

XXI BMIC – Brazilian Meeting on Inorganic Chemistry and X BMRE – Brazilian Meeting on Rare Earths - (Room 1B – Main Floor)

13:00 – 19:00	Reception - Registration
19:00	Opening Ceremony
19:30 – 20:30	Opening Conference <i>Chair: Fernando Sigoli</i> Frank Erich Osterloh (University of California, USA) <i>“Inorganic Materials for Photochemical and Photovoltaic Solar Energy Conversion”</i>
20:30 – 00:00	Welcome Party

Friday – September 13th

	Room 1B (Main Floor)	Room 301 (3 rd Floor)	Room 1A (2 nd Floor)	Room 2A (4 th Floor)
8:30 – 10:00	Sponsors Talk (8:30 am) <i>How to Publish: A successful submission process to favour your article publication</i> (Elizabeth Magalhães - Royal Society of Chemistry) Chair: Maria Helena Araújo	Mini-course 1 <i>Simultaneous Fluorescence and absorbance spectroscopy (Horiba)</i>	Mini-course 2 <i>LS and jj spectroscopy terms and spectroscopy terms for small molecules. (Roberto B. Faria-UFRJ)</i>	Mini-course 3 <i>The basics on Sci-Finder and how to publish your next scientific article (ACS)</i>
10:00 – 10:30	Coffee Break			
10:30 – 11:20 (50 min)	Maribel Navarro (Universidade Federal de Juiz de Fora) <i>"Metallo drugs: a multi-target approach to the treatment of parasitic diseases"</i> Chair: Victor Deflon		Marius Andruh (University of Bucharest, Romania) <i>"Magnetic and Luminescent Molecular Materials Constructed from Lanthanides - New Synthetic Approaches."</i> Chair: Guilherme Pereira Guedes	Deryn Fogg (University of Ottawa, Canada) <i>"Olefin Metathesis for the 21st Century: Decomposition Guides Design."</i> Chair: Eduardo Nicolau
11:20 – 12:10 (50 min)	Júlio Santos Rebouças (Universidade Federal da Paraíba, Brazil) <i>"Zn(II) porphyrins as photosensitizers: The good, the bad, and the ugly."</i> Chair: Victor Deflon		Christopher L. Cahill (Columbian College of Arts & Sciences, USA) <i>"Non-covalent interactions for assembly and energy transfer within f-element hybrid materials."</i> Chair: Fernando Sigoli	Cynthia Lopes (Universidade Federal de Minas Gerais, Brazil) <i>"Oxamate complexes as candidates for spin qubits: challenges and perspectives."</i> Chair: Eduardo Nicolau
12:10 – 14:00	Lunch			
14:00 – 14:30 (30 min)	Annie Castonguay (INRS-Centre Armand-Frappier Santé Biotechnologie, Université du Québec, Canada) <i>"Biological activity of ruthenium-based organometallic complexes."</i> Chair: Luiz Antonio S. Costa		Gael Ung (University of Connecticut, USA) <i>"Hot and cold circularly polarized luminescence with molecular f-element complexes."</i> Chair: Fernando Sigoli	Edmond Gravel (Frederic Joliot Institute for life science, France) <i>"Carbon nanotube-supported metals for heterogeneous catalysis."</i> Chair: Maria Helena Araujo
14:30 – 15:00 (30 min)	Vânia Denise Schwade (Universidade Federal de Santa Maria, Brazil) <i>"Metal complexes of chromone and coumarin-containing molecules – on the structure and properties investigation."</i> Chair: Marciela Scarpellini		Paulo Cesar de Sousa Filho (Universidade Estadual de Campinas, Brazil) <i>"Luminescence meets catalysis in rare earth vanadate nanoparticles".</i> Chair: Fernando Sigoli	André Sarto Polo (Universidade Federal do ABC, Brazil) <i>"Enhancing Perovskite Solar Cells Durability via Compositional and Dimensional Strategies."</i> Chair: Maria Helena Araujo
15:00 – 16:00	Special Section: BWIC – Brazilian Women in Inorganic Chemistry			
16:00 – 16:30	Coffee Break			
16:30 – 17:30 (3 min) each	Flash Presentation 1 Chair: Heveline Silva			
17:30 – 19:30	Poster Session 1			

Saturday – September 14th

	Room 1B (Main Floor)	Room 301 (3 rd Floor)	Room 1A (2 nd Floor)	Room 2A (4 th Floor)
8:30 – 10:00	Triple-Helix Session <i>(Government, Industry and University)</i> <i>"Exploration and Regulation of Rare Earth Elements or Critical Materials in Brazil and Around the World."</i>	Mini-course 1 <i>Simultaneous Fluorescence and absorbance spectroscopy (Horiba)</i>	Mini-course 2 <i>LS and jj spectroscopy terms and spectroscopy terms for small molecules. (Roberto B. Faria-UFRJ)</i>	Mini-course 3 <i>The basics on Sci-Finder and how to publish your next scientific article (ACS)</i>
10:00 – 10:30	Coffee Break			
10:30 – 11:20 <i>(50 min)</i>	Justin Wilson (University of California-Santa Barbara, USA) <i>"Design Strategies for Radiometal Chelation in Nuclear Medicine."</i> <i>Chair: Luiz Antônio S. Costa</i>		Eva Hemmer (University of Ottawa, Canada) <i>"Architectural Control of Lanthanide-based Nanoparticles: from Potential Multimodal Imaging Probes to Miniature Thermometers."</i> <i>Chair: Fernando Sigoli</i>	Holger Braunschweig (University of Würzburg, Germany) <i>"Borametallomimetics - can Boron act as a Transition Metal?"</i> <i>Chair: Eufrânio Nunes S. Jr</i>
11:20 – 12:10 <i>(50 min)</i>	Camilla Abbehausen (Universidade Estadual de Campinas, Brazil) <i>"Metallo drugs as Alternatives for the Therapy of Neglected Tropical Diseases."</i> <i>Chair: Luiz Antônio S. Costa</i>		Eva Rentschler (Johannes Gutenberg University, Germany) <i>"Metallacrown complexes: host-guest interaction paving the way for molecular magnets."</i> <i>Chair: Guilherme Pereira Guedes</i>	Michael Zaworotko (University of Limerick, Ireland) <i>"Materials for a Sustainable World."</i> <i>Chair: Javier Elena</i>
12:10 – 12:20	Group-Photo (CAD 1 entrance)			
12:20 – 14:00	Lunch			
14:00 – 14:40 <i>(40 min)</i>	<i>Chair: Maribel Navarro</i> Lena Ruiz-Azuara (Universidad Nacional Autónoma de Mexico, Mexico) <i>"Antineoplastic and antiparasitic metallo drugs based on a facultative ligand pdto(N₂S₂) with its O and Se analogues."</i>		<i>Chair: Ernesto S. Lang</i> Peter Junk (James Cook University, Australia) <i>"Recent developments in redox transmetalation chemistry involving rare earth metals."</i>	<i>Chair: Maria Helena de Araujo</i> Ana Flávia Nogueira (Universidade Estadual de Campinas, Brazil) <i>"Challenges with metal halide perovskites solar cells: what we have learned so far."</i>
14:40 – 15:00 <i>(20 min)</i>	Camila Anchau Wegermann (Universidade Estadual do Rio de Janeiro, Brazil) <i>"Prospecting the biological and catalytic activity of nitroxide radical derivatives and their complexes."</i>		Airton Germano Bispo Junior (Universidade de São Paulo, Brazil) <i>"Pushing the Limits of Slow Magnetic Relaxation and Luminescence Thermometry in Multifunctional Lanthanide(III) Complexes."</i>	Joshua Telser (Roosevelt University, USA) <i>"The Remarkable Chemistry of Titanium and Vanadium as Supported by Spectroscopy."</i>
15:00-15:20 <i>(20 min)</i>	Pedro Ivo da Silva Maia (Universidade Federal do Triângulo Mineiro, Brazil) <i>"Gold(I) based metallacycles and metallacages with bipodal ligands: from homo to heterometallic assemblies."</i>		Beate Saegesser Santos (Universidade Federal de Pernambuco – UFPE, Brazil) <i>"Silver Nanoplatelets as new tools for Efficient Photodynamic Inactivation of Microorganisms."</i>	Sérgio Antônio Marques de Lima (Universidade Estadual Paulista, Presidente Prudente, Brazil) <i>"Exploring the Luminescence of Iridium Complexes: From Basic Photophysics to Bioimaging and Solid State Lighting Applications."</i>
15:20 – 16:00 <i>(10 min) each</i>	Short Lectures 1 – 4 <i>Chair: Juliana Fedoce</i>		Short Lectures 5 – 8 <i>Chair: Rogéria Rocha Gonçalves</i>	Short Lectures 9 – 12 <i>Chair: Célia Machado Ronconi</i>
16:00 – 16:30	Coffee Break			
16:30 – 17:30 <i>(3 min) each</i>	Flash Presentation 2 <i>Chair: Heveline Silva</i>			
17:30 – 19:30	Poster Session 2			

Sunday - September 15 th				
	Room 1B (Main Floor)	Room 301 (3 rd Floor)	Room 1A (2 nd Floor)	Room 2A (4 th Floor)
8:30 – 10:00	Sponsors Talk <i>Midas/Escalab Granioter Instituto Sua Ciência</i>	Mini-course 1 <i>Simultaneous Fluorescence and absorbance spectroscopy (Horiba)</i>	Mini-course 2 <i>LS and jj spectroscopy terms and spectroscopy terms for small molecules. (Roberto B. Faria-UFRJ)</i>	Mini-course 3 <i>The basics on Sci-Finder and how to publish your next scientific article (ACS)</i>
10:00 – 10:30	Coffee Break			
10:30 – 11:00 <i>(30 min)</i>	Fabio Doctorovich (Universidad de Buenos Aires, Argentina) <i>"Endogenous and Exogenous Generation of Nitroxyl (HNO)."</i> <i>Chair: William R. Rocha</i>	Moritz-Kühnel (University of Hohenheim, Germany) <i>"Solar-driven generation of sustainable feedstocks from water, waste and CO₂."</i> <i>Chair: Ernesto S. Lang</i>	Richard Walton (University of Warwick, UK) <i>"Stable Metal-Organic Frameworks for Applications in Heterogeneous Catalysis in Energy and Sustainability."</i> <i>Chair: Willian Xerxes</i>	
11:00 – 11:30 <i>(30 min)</i>	Sofia Nikolaou (Universidade de São Paulo, Ribeirão Preto, Brazil) <i>"Investigating polynuclear ruthenium acetate properties of biological interest."</i> <i>Chair: William R. Rocha</i>	Fiorenzo Vetrone (Université du Québec, Canada) <i>"Applications of Luminescent Rare Earth Doped Nanoparticles in Nanomedicine."</i> <i>Chair: Fernando Sigoli</i>	Fausthon Fred da Silva (Universidade Federal da Paraíba, Brazil) <i>"Boosting the Electrocatalytic Activity of Metal-Organic Frameworks Derived Metal-Oxide Nanoparticles in Oxygen Evolution Reaction."</i> <i>Chair: Willian Xerxes</i>	
11:30 – 12:20 <i>(3 min) each</i>	Flash Presentation 3 <i>Chair: Heveline Silva</i>			
12:20 – 14:00	Lunch			
14:00 – 16:00	Poster Session 3			
16:00 – 16:30	Coffee Break			
16:30 – 17:10	Early Career Award Lecture Royal Society of Chemistry and Sociedade Brasileira de Química <i>Chair: Bernardo A. Iglesias / Elizabeth Magalhães</i>			
17:10 – 18:00	Closing Lecture Nicholas P. Farrell (Virginia Commonwealth University, USA) <i>"Medicinal Inorganic Chemistry. Evolving the understanding of anticancer mechanism of platinuns"</i> <i>Chair: Ana Paula Soares Fontes</i>			
18:00 – 19:00	Closing ceremony – Awards – DQI Assembly			
19:00	Farewell Party			