

XXI Brazilian Symposium on Theoretical Chemistry (SBQT)

Scientific Program

Monday (11/08)	
10:00-10:30	Opening Session Chair: Willian R. Rocha
10:30-11:30	Plenary Lecture 1 Sylvio Canuto Universidade de São Paulo - USP <i>“Theoretical Studies of Molecular Spectroscopy in Simple Liquids and Complex Environments”</i>
11:30-14:00	Lunch Chair: José Walkimar de Mesquita Carneiro - UFF
14:00-14:40	Invited Lecture 1 Josefredo R. Pliego Jr. Universidade Federal de São João del-Rei - UFSJ <i>“Beyond the Solvent Effect: Theoretical Design of Nanostructured Environment for Controlling Ionic Reactions”</i>
14:40-15:20	Invited Lecture 2 Elizete Ventura do Monte Universidade Federal da Paraíba - UFPB <i>“Photophysical study of solute-solvent energy transfer”</i>
15:20-16:00	Invited Lecture 3 Ricardo Oliveira Freire Universidade Federal de Sergipe - UFS <i>“Development and application of methods and software for the study of luminescent nanomaterials for application as chemical sensors and markers”</i>
16:00-16:30	Interval Chair: João Paulo Ataíde Martins - UFMG
16:30-16:45	Oral Presentation 1 Tiago Vinícius Alves Universidade Federal da Bahia - UFBA <i>“Differences in the torsional anharmonicity between reactant and transition state: the case of 3-butenal + H abstraction reactions”</i>
16:45-17:00	Oral Presentation 2 Alex Bispo Gama Universidade Estadual de Goiás - UEG <i>“Interpretação da Cinética Super-Arrhenius em Processos Biológicos: Incorporação da Relação de Kramers-Stokes-Einstein”</i>
17:00-17:15	Oral Presentation 3 Carlos Vital dos Santos Júnior Universidade Federal do Rio Grande do Norte - UFRN <i>“Analysis of chemical bonds in $S_N2@C$ and $@Si$ reactions mechanisms in the gas phase”</i>

17:15-17:30	Oral Presentations Q&A Session
17:30-18:30	Poster Session 1

Tuesday (11/09)	
Chair: André Farias de Moura - UFSCAR	
9:00-9:40	Invited Lecture 4 Alejandro Toro-Labbé Pontificia Universidad Católica de Chile - Chile <i>“Unveiling the Mystery of Reaction Mechanisms”</i>
09:40-10:30	Plenary Lecture 2 Maria João Ramos Universidade do Porto - Portugal <i>“Biodegrading Plastic”</i>
10:30-11:10	Invited Lecture 5 Bruno Araújo C. Horta Universidade Federal do Rio de Janeiro - UFRJ <i>“Software Tools for Force-Field Development”</i>
11:10-12:00	Plenary Lecture 3 Matthias Bickelhaupt Vrije Universiteit Amsterdam - Netherlands <i>“Paradigm Shifts in the Theory of Chemical Structure and Reactivity”</i>
12:00-14:00	Lunch
14:00-16:00	Especial Session 40 years of SBQT Chair: Marco Antônio Chaer do Nascimento Universidade Federal do Rio de Janeiro - UFRJ
16:00-16:30	Interval
Chair: Renaldo Tenório Moura Júnior - UFPB	
16:30-16:45	Oral Presentation 4 Leonardo Baptista Universidade do Estado do Rio de Janeiro - UERJ <i>“Estudo da Decomposição Térmica do Sistema H₂O₂/H₂O e Suas Aplicações na Indústria Aeroespacial”</i>
16:45-17:00	Oral Presentation 5 Paulo Henrique Ribeiro Amaral Universidade de São Paulo - USP <i>“Positron binding to atoms and molecules: Machine learning studies”</i>
17:00-17:15	Oral Presentation 6 Tiago Espinosa de Oliveira Universidade Federal de Ciências da Saúde de Porto Alegre - UFCSPA <i>“Estudos computacionais da poli(N-isopropilacrilamida) em solução aquosa de glicerol”</i>
17:15-17:30	Oral Presentations Q&A Session
17:30-18:30	Poster Session 2

Wednesday (11/10)	
	Chair: Itamar Borges Junior - IME
9:00-9:40	Invited Lecture 6 Annika Bande Helmholtz-Zentrum Berlin - Germany <i>"The Fascinating Journeys of Electrons in the Realm of Nanostructures"</i>
09:40-10:30	Plenary Lecture 4 Feliu Maseras Institut Català d'Investigació Química - Spain <i>"How does microkinetic modeling bring DFT closer to experiment ?"</i>
10:30-11:10	Invited Lecture 7 Luis Guilherme C. Rego Universidade Federal de Santa Catarina - UFSC <i>"Spin-Dependent Transport in Chiral Molecular Wires"</i>
11:10-12:00	Plenary Lecture 5 Frank Neese Max-Planck Institut Für Kohlenforschung - Germany <i>"How Nature Activates the C-H Bond in Methane: Lessons from a Combination of Spectroscopy and Quantum Chemistry"</i>
12:00-14:00	Lunch
	Chair: Guilherme Ferreira de Lima - UFMG
14:00-14:40	Invited Lecture 8 Antônio José Roque Centro Nacional de Pesquisa em Energia e Materiais <i>"O CNPEM e a nova Fonte de Luz Síncrotron Brasileira, Sirius"</i>
14:40-15:20	Invited Lecture 9 Giovanni F. Caramori Universidade Federal de Santa Catarina - UFSC <i>"Automative Quantum Chemical Microkinetic Simulations for Complex Chemical Reactions"</i>
15:20-16:00	Invited Lecture 10 Ataulpa A. C. Braga Universidade de São Paulo - USP <i>"Novel Ni-catalyzed C-C and C-O coupling reactions: a computational approach"</i>
16:00-16:30	Interval
	Chair: Hubert Karl Stassen - UFRGS
16:30-16:45	Oral Presentation 7 Gabriel Urquiza Universidade Federal de Pernambuco - UFPE <i>"An Uncomplicated but Effective Force Field for the Pre-optimization of Geometries of Metal Complexes for Quantum Chemical Calculations"</i>
16:45-17:00	Oral Presentation 8 Yuro Alexandre Aoto Universidade Federal do ABC - UFABC

	“A geometric interpretation for coupled-cluster theory being more accurate than corresponding configuration interaction”
17:00-17:15	Oral Presentation 9 Kalil Bernardino Universidade de São Paulo - USP “Role of coulomb interactions and density on the viscosity and non-newtonian behavior of ionic liquids - a molecular dynamics study”
17:15-17:30	Oral Presentations Q&A Session
17:30-18:30	Poster Session 3

Thursday (11/11)	
9:00-9:20	Alfredo Mayall Simas Universidade Federal de Pernambuco - UFPE Introdução à Sessão Especial: <i>Computação Quântica e Inteligência Artificial em Química Teórica</i>
09:20-9:50	Round Table: <i>Quantum Computing and Artificial Intelligence in Theoretical Chemistry</i> Chair: Alfredo Mayall Simas Debaters: Alán Aspuru-Guzik - University of Toronto - Canada Pavlo Dral - Xiamen University - China Juarez L. F. da Silva - Universidade de São Paulo - USP
09:50-10:40	Plenary Lecture 6 Alán Aspuru-Guzik University of Toronto - Canada “There is no time for science as usual”
10:40-11:30	Plenary Lecture 7 Pavlo Dral Xiamen University - China “Quantum Chemistry Assisted by Machine Learning”
11:30-12:10	Invited Lecture 11 Juarez L. F. da Silva Universidade de São Paulo - USP “Challenges to Combine Quantum Chemistry, Machine Learning, and Data Mining Techniques to the Study and Design of Molecular Systems”
12:10-14:00	Lunch
	Chair: Kelson Mota Teixeira de Oliveira - UFAM
14:00-14:40	Invited Lecture 12 Sergey Varganov University of Nevada - USA “Modeling Kinetics and Dynamics of Spin-Dependent Processes”
14:40-15:20	Invited Lecture 13 Jaroslav Burda Charles University - Czech Republic “Electronic excited states of conjugated molecules and their lifetimes”

15:20-16:00	Invited Lecture 14 Breno R. L. Galvão Centro Federal de Educação Tecnológica de Minas Gerais - CEFET-MG <i>“Chemistry in the Interstellar medium”</i>
16:00-16:30	Interval
	Chair: Dalva Ester da Costa Ferreira - UFVJM
16:30-16:45	Oral Presentation 10 Graziâni Candiotto Universidade Federal do Rio de Janeiro - UFRJ <i>“OLEDs de Alq₃ dopado com DCM2: desvio para o vermelho causado pelo efeito stark não linear e pela difusão de excitons mediada por Förster”</i>
16:45-17:00	Oral Presentation 11 Maicon Lourenço Universidade Federal do Espírito Santo - UFES <i>“Advances on Active Learning for Efficient Global Optimization of Atomic Clusters”</i>
17:00-17:15	Oral Presentation 12 Leonardo Dos Santos Universidade Federal de Minas Gerais - UFMG <i>“Electron-Density Polarization Effects in Molecular Crystals and Bioactive Environments”</i>
17:15-17:30	Oral Presentations Q&A Session
17:30-18:30	Poster Session 4

Friday (11/12)	
	Chair: Demétrio Antônio da Silva Filho - UNB
9:00-9:40	Invited Lecture 15 Glória Cárdenas-Jíron Universidade de Santiago de Chile - Chile <i>“Tuning the Visible/Near-Infrared Optical Properties and Charge Transport of Porphyrins and Phthalocyanines”</i>
09:40-10:30	Plenary Lecture 8 Márcia C. Barbosa Universidade Federal do Rio Grande do Sul - UFRGS <i>“Water: from the Ice Age to the Carbon Nanotubes”</i>
10:30-11:10	Invited Lecture 16 Victor Batista Yale University - USA <i>“Studies of PCET in Natural and Artificial Photosynthesis”</i>
11:10-11:50	Invited Lecture 17 José Rachid Mohallem Universidade Federal de Minas Gerais - UFMG <i>“Benchmark Spectroscopic Linelists of Primordial Molecules for Astrophysics and Astrochemistry”</i>

11:50-14:00	Lunch
	Chair: Heitor Avelino de Abreu - UFMG
14:00-14:40	Invited Lecture 18 Teodorico C. Ramalho Universidade Federal de Lavras - UFLA <i>"Innovation and opportunities toward new molecules for the agrochemical industry: from theory to technology"</i>
14:40-15:20	Invited Lecture 19 Carolina Horta Andrade Universidade Federal de Goiás - UFG <i>"Artificial Intelligence-Assisted Drug Discovery for Neglected and Emerging Diseases"</i>
15:20-16:00	Oral Presentations of Sponsors: Seagate Versatus
16:00-16:30	Interval
16:30-18:30	Closing Session