International Symposium on Multi-Scale Simulation of Condensed-Phase Reacting Systems - MSCRS2016
Nagoya University – Japan

PROGRAM

Monday, Oct 10th

13:30 Registration Desk Open

NU Workshop

"Current Challenges and Advances in Understanding of Chemical Reaction in Condensed System via Theoretical Approaches"

14:20-14:30 **Opening**

Session NU1 - Quantum Chemistry Calculations of Molecular Properties
Chair: M. Nakata (RIKEN)

14:30-15:00 L1-01 **Manuel A. Aguilar** (Univ. of Extremadura)
Some Examples of the Application of the Mean Field Approximation to the Study of Solvent Effects

15:00-15:30 L1-02 **Vincent Robert** (Univ. of Strasbourg)
Strategies for Large-System Electronic Structures

15:30-16:00 L1-03 **Satoru Iuchi** (Nagoya Univ.)
Molecular Dynamics Simulation of Light-Induced Spin Crossover in $[Fe(bpy)_3]^{2+}$

16:00-16:30 **BREAK**

Session NU2 - Theoretical Chemistry and Development of Methodology
Chair: T. Yamamoto (Kyoto Univ.)

16:30-17:00 L1-04 **Sangyoub Lee** (Seoul Nat. Univ.)
Perspectives on the Diffusion-Influenced Bimolecular Reaction Kinetics

17:00-17:30 L1-05 **M. Elena Martín** (Univ. of Extremadura)
Theoretical Study of the Photoactive Yellow Protein Chromophore Excited State in Water Solution

17:30-17:50 L1-06 **Sergi Vela Llausí** (Univ. of Strasbourg)
Spin and Phase Transitions in Fe(II)-Based Architectures

17:50-18:20 L1-07 **Carmen Domene** (King's College London)
Understanding Transport and Reactivity in Proteins by Multiscale Simulation

Tuesday, Oct. 11th

09:00 Registration Desk Open

JSPS-FAPESP Joint Research Workshop

"Overseas Challenges in Photochemical and Photobiological Sciences via Computational and Experimental Approaches"

09:20-09:50 Opening

Session JB1 - Photoabsorption and Photoemission
Chair: S. Canuto (Univ. of São Paulo)

09:50-10:20 L2-01 **Kaline Coutinho** (Univ. of São Paulo)
Theoretical Studies of the Photo-Absorption and -Emission of Molecules in Solution

10:20-10:50 L2-02 **Nobuaki Koga** (Nagoya Univ.)
Theoretical Study of Photoabsorption and Emission of Firefly-Bioluminescence-Related Molecules

10:50-11:20 **BREAK**

Session JB2 –Surface-Enhanced Spectroscopy, Ionic Liquids, Interfaces and Batteries
Chair: N. Koga (Nagoya Univ.)

11:20-11:50 L2-03 **Diego Pereira dos Santos** (Univ. of Campinas)
Surface-Enhanced Raman Scattering as a Probe of Metal Nanoparticle Properties

11:50-12:10 L2-04 **Kenta Motobayashi** (Nagoya Inst. of Tech.)
Interfacial Structure of Ionic Liquids near Metal Electrodes: Hysteretic Potential Dependence Studied by Surface-Sensitive Spectroscopy

12:10-12:30 L2-05 **Norio Takenaka** (Nagoya Univ.)
Theoretical Study on Solid Electrolyte Interphase (SEI) Film Formation in Secondary Batteries

12:30-14:00 **OFFICIAL PHOTO**
LUNCH

Session JB3 - Development of Methods in Theoretical Chemistry
Chair: A. Nakayama (Hokkaido Univ.)

14:00-14:30 L2-06 **Hirofumi Sato** (Kyoto Univ.)
Molecular Theory of Chemical Processes in Condensed Phase

14:30-15:00 L2-07 **Rogério Custodio** (Univ. of Campinas)
Some Perspectives of Accurate Calculations Based on Composite Methods

15:00-15:20 L2-08 **Daisuke Yokogawa** (Nagoya Univ.)
New Electrostatic Potential Charge Including Spatial Electron Density Distribution

15:20-15:40 L2-09 **Yue Chen** (Hokkaido Univ.)
Coordination Strategy to Realize Sextuply Bonded Complex. Theoretical Prediction

15:40-16:00 L2-10 **Yukichi Kitamura** (Nagoya Univ.)
Dual Approach to Vibrational Spectra in Solution: Microscopic Influence of Hydrogen Bonding to the State of Motion of Glycine in Water

16:00-16:30 **BREAK**

Session JB4 – Catalyzed Reactions Applied to Organic and Metallic Compounds
Chair: H. C. Georg (Fed. Univ. of Goiás)

16:30-16:50 L2-11 **Marco A. Barbosa Ferreira** (Fed. Univ. of São Carlos)
New Strategies in Preparation of Substituted Cyclic Compounds

16:50-17:10 L2-12 **Ricardo S. Schwab** (Fed. Univ. of São Carlos)
Magnetic Nanoparticles: an Efficient Support for Immobilization of Transition-Metals

17:10-18:30 **POSTER SESSION**

18:30-20:30 **WELCOME RECEPTION PARTY**

Wednesday, Oct. 12th

08:45 Registration Desk Open

Session JB5 – Complex Systems and Polymerization
Chair: R. Custodio (Univ. of Campinas)

09:00-09:30 L3-01 **Akira Nakayama** (Hokkaido Univ.)
Catalytic Reactions at the Water/Ceria Interface: Role of the Acid-Base Sites

09:30-09:50 L3-02 **Leandro Martínez** (Univ. of Campinas)
Conformational Dynamics of the Nuclear Receptor Switch of Transcription Activation: Simulation of Free-Energy Landscapes and Time-Dependent Fluorescence Anisotropy Decays

09:50-10:10 L3-03 **Gustavo Troiano Feliciano** (São Paulo State Univ.)
Computer Modeling of Complex Processes Using Multiscale Atomistic/Electronic Structure Simulation Methods

10:10-10:30 L3-04 **Hadi Arefi** (Kyoto Univ.)
Supramolecular Polymerization of SOPV Monomers: A Molecular Dynamics Study of Dimerization/Tetramerization Mechanism and Beyond

10:30-10:50 L3-05 **Masayoshi Takayanagi** (Nagoya Univ.)
Theoretical Study on Behaviors of Host PCP and Guest Methyl Methacrylate toward Understanding Tacticity Control Mechanism

10:50-11:20 **BREAK**

Session JB6 – Applications to Solar Cells
Chair: H. Sato (Kyoto Univ.)

11:20-11:50 L3-06 **Kumi Yoshida** (Nagoya Univ.)
Photochemical Property of Anthocyanins: from Flower Coloration toward Dye-Sensitized Solar Cell

11:50-12:10 L3-07 **Paula Homem de Mello** (Fed. Univ. of ABC)
DFT Studies on Dyes for Photodynamic Therapy and Solar Cells

12:10-12:30 L3-08 **Marina Sparvoli de Medeiros** (Fed. Univ. of ABC)
Synthesis and Deposition of Graphene Oxide Films for Solar Applications”

12:30-14:00 **LUNCH**

Session JB7 - Photochemistry and Photobiology
Chair: K Coutinho (Univ. of São Paulo)

14:00-14:30 L3-09 **Akiyoshi Hishikawa** (Nagoya Univ.)
Reaction Microscope: Real-time Imaging of Ultrafast Molecular Dynamics

14:30-15:00 L3-10 **Herbert C. Georg** (Fed. Univ. of Goiás)
Using the ASEC-FEG Method to Study Electronic Properties of Molecules

15:00-15:20 L3-11 **Carlos Bistafa** (Nagoya Univ.)
Combining Sequential-QM/MM and Free Energy Gradient Methods to Obtain Excited State Geometries in Solvent at Reasonable Computational Cost

15:20-15:40 L3-12 **Yu Harabuchi** (Hokkaido Univ.)
Systematic Exploration of Internal Conversion and Intersystem Crossing Pathways: Toward Prediction of Fluorescence Quantum Yields

15:40-16:00 L3-13 **Kenichiro Saita** (Hokkaido Univ.)
Theoretical Study on the Photoreactivity of fac-$[Re^{I}(bpy)(CO)_3(PR_3)]^+$ Complex

16:00-16:30 **BREAK**

16:30-17:30 **COMPREHENSIVE DISCUSSION:**
Future Challenges and Overseas Collaborations, via Theoretical, Experimental, and Computational Approaches

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Thursday, Oct. 13th

JSPS-FAPESP Official Site Visit to FIFC (Kyoto)