

PROGRAM



CRC-EC Joint International Symposium on Chemical Theory for Complex Systems

January 9-10, 2014, Emory University, Atlanta, USA



**Emerson
Center (EC)**

Harland Cinema

Organizer:

C. L. Emerson Center (EC) for Scientific Computation (Emory University, USA)
Catalysis Research Center (CRC), Hokkaido University, Japan)

Co-Organizer: Fukui Institute for Fundamental Chemistry (Kyoto, Japan)

Organizing Committee:

Kiyotaka Asakura (Hokkaido, Japan)

Joel M Bowman (Emory, USA)

Francesco Evangelista (Emory, USA)

Jun-ya Hasegawa (Hokkaido, Japan)

James T. Kindt (Emory, USA)

Jamal Musaeov (Emory, USA)

Shigeyoshi Sakaki (Kyoto, Japan)

Koichi Yamashita (Tokyo, Japan)

Co-Sponsors:

**Department of
Chemistry (Emory)**



The Hightower Foundation (Emory)

January 9, 2014

Chair: Jamal Musaev (Emory University)

- 9:00- 9:10 Opening Address from the Director of Emerson Center: **Jamal Musaev**
9:10- 9:20 Welcome Address from the Dean of Emory College of Arts and Sciences: **Robin Forman**
9:20- 9:30 Opening Address from the Director of Catalysis Research Center: **Atsushi Fukuoka**
9:30- 9:40 Emerson Center Lectureship Award Presentation: **Kurt Warncke**

9:40-10:25 **Keiji Morokuma** (Kyoto University; Emory University)
Chemical Theory of Complex Molecular Systems: Discovery and Insights from Computational Studies of Chemical Reactions

10:25-10:50 **Qiang Cui** (University of Wisconsin)
Multi-Scale Computational Analysis of Biomolecular Actions

----- 10:50 - 11:10 Coffee Break -----

Chair: M. Aida (Hiroshima University)

- 11:10-11:55 **William H. Miller** (University of California, Berkeley)
Semiclassical Theory of Electronically Non-Adiabatic Dynamics
11:55-12:30 **Kazuo Takatsuka** (Institute for Molecular Science; The University of Tokyo)
Progress in Time Dependent Quantum Chemistry
12:30-12:55 **Akira Nakayama** (Hokkaido University)
Photophysics of Pyrimidine Nucleobases
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Chair: M. Heaven (Emory University)

- 14:15-15:00 **George C. Schatz** (Northwestern University)
Coupling Quantum Mechanics to Classical Electrodynamics
15:00-15:35 **Joel M. Bowman** (Emory University)
*I. Vibrational Relaxation Dynamics of Clusters from (HCl)₃ to Bulk Water;
II. A "Paper and Pencil" Theory of Mode-Specific Tunneling, Tested for Malonaldehyde and Applied to cis-HOCO*
15:35-16:10 **Koichi Yamashita** (The University of Tokyo)
Electron Transfer and Thermal Transport at Surfaces/Interfaces

----- 16:10 - 16:30 Coffee Break -----

Chair: K. Asakura (Hokkaido University)

- 16:30-17:05 **Per E. M. Siegbahn** (Stockholm University)
The Mechanisms for Water Oxidation in Photosystem II
- 17:05-17:30 **Shigehiko Hayashi** (Kyoto University)
Crucial Role of Protein Flexibility in Enzymatic Catalysis
- 17:30-17:55 **James Kindt** (Emory University)
Thermodynamics of Cluster Formation from Simple Simulations
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- 19:00 *Banquet (@ Emory Conference Center Hotel, by Invitation only)*

January 10, 2014

9:00-11:30 **Poster Session**

Chair: J. Musaev (Emory University)

- 13:00-13:35 **Hiroshi Nakatsuji** (Quantum Chemistry Research Institute)
Schrödinger Equation and Pauli Principle Governing Chemistry
- 13:35-14:00 **C. David Sherrill** (Georgia Institute of Technology)
Non-Covalent Interactions in Complex Systems
- 14:00-14:25 **Francesco Evangelista** (Emory University)
TBA

----- 14:25-15:00 *Coffee Break* -----

Chair: S. Sakaki (Kyoto University)

- 15:00-15:45 **William A. Goddard, III** (California Institute of Technology)
First-Principles Based Multiscale Multiparadigm Methods for Applications to Complex Systems
- 15:45-16:20 **Tom Ziegler** (University of Calgary)
Constricted Variational Density Functional Theory. A New DFT Approach to the Study of Excited States
- 16:20-16:45 **Rigoberto Hernandez** (Georgia Institute of Technology)
Including Roaming Trajectories within the TST Fold
- 16:45-17:00 **Concluding Remarks: Shigeyoshi Sakaki (Kyoto University)**
- 18:30** *Banquet (@ Winship Ballroom, DUC, by Invitation only)*