第69回岡崎コンファレンス New Frontier in Quantum Chemical Dynamics

昨今様々な分野において量子効果を利用した分子機能の利用や提案が活発に報告されている。このような状況を踏まえ、化学動力学分野における最新の研究を行っている研究者が集い、量子効果の扱いと制御という枠組みの中で最新の研究結果、手法、傾向等について議論することを目的とした岡崎コンファレンス New Frontier in Quantum Chemical Dynamics「量子化学動力学の最先端」を2010年2月21日(日)～23日(火)に開催した。

国内外の理論・実験研究者を迎え、合計32件の招待講演（海外8名）からなるオーラルセッションのみで討論を行った。事前登録参加者数が80名、当日の申し込みの参加者を加えると総参加者数は100名程度であった。Welcome partyでは、中村所長や海外から？差し入れがあったりして、おかげさまで赤字にならずに運営できたのは助かった。

3日間で32件の口頭発表を行ったため、かなり過密スケジュールとなった。特に、活発な議論のため、3日目の午前のセッションがだいぶ押してしまった。海外研究者との昼食を会場近くの一色屋でとっていたが、会場に時間どおり戻れず、座長及び講演者の方にご迷惑をかけてしまい反省している。海外の研究者を迎えるにあたってビザや旅費関係の手続きでも苦労があったが、その先生方からも大変良かったと高い評価を受けられたのは幸いである。国内外の今後の化学動力学の進展に微かながらでも役立ったかと思うと喜びもひとしおである。

最後に素晴らしいハプニングが懇親会にて起こったことをここに紹介したい。それは図らずも、Aquilanti博士からの量子化学動力学分野におけるこれまでの中村宏樹先生のご貢献に対する感謝のお言葉が述べられたことが切掛けとなり、参加者が次々感謝の言葉を述べられたことである。今回のコンファレンスは退職記念として開催されたわけではなかったが、中村先生のこれまでのこの分野へのご貢献を考えると、ハプニングとしてはとてもよかったのではないかと思う。

（世話人　南部 伸孝、石田 俊正、
小杉 信博、信定 克幸）

The 69th Okazaki Conference on New Frontier in Quantum Chemical Dynamics, Feb.21-23,2010

The 69th Okazaki Conference on "New Frontier in Quantum Chemical Dynamics"

February 21 (Sun.)

9:00-9:10 Opening address(Hiroki Nakamura, Director General, IMS)
9:10-9:20 Introductory talk (Shinkoh Nanbu, Sophia Univ.)

Session 1. Basic Theory and Concepts of Chemical Dynamics

Chairperson: Kazuo Takatsuka

9:20-9:55 **Hiroki Nakamura** (Institute for Molecular Science) "Semiclassical Theories of Quantum Effects in Chemical Dynamics – From Comprehension to Control of Dynamics"
9:55-10:30 **Vincenzo Aquilanti** (Università di Perugia) "Hyperspherical and related views at elementary chemical processes"

Chairperson: Toshiyuki Takayanagi

10:50-11:25 **Kazuo Takatsuka** (University of Tokyo) "Nuclear semiclassics and nonadiabatic electron dynamics in molecules"
11:25-12:00 **Shinnosuke Kawai** (Hokkaido University) "Nonlinear Dynamics of Chemical Reactions through a Saddle Point"

Session 2. Quantum dynamics and Non-adiabatic Processes

Chairperson: Tetsuya Taketsugu

13:30-14:05 **Satoshi Yabushita** (Keio University) "On the use of complex optimized GTOs for the efficient calculations of resonance state energies and photoionization cross-sections"
14:05-14:40 **Hiroshi Ushiyama** (University of Tokyo) "Proton Transfer Dynamics"
14:40-15:15 **Kenji Honma** (Hyogo University) "Reaction dynamics of transition metal atoms studied by crossed beam technique"
15:15-15:50 **Ikuo Tokue** (Niigata University) "Dissociation Dynamics After the SO2(C 1B2¬X 1A1) Excitation Studied by Wave Packet Propagation Technique"

Chairperson: Toshimasa Ishida

16:10-16:45 **Takeshi Yamamoto** (Kyoto University) "Some numerical quests for accurate quantum dynamics in gas and condensed phases"
16:45-17:20 **Haruki Ishikawa** (Kobe University) "Infrared spectroscopy of jet-cooled tautomeric dimer of 7-azaindole: A model system for the ground-state double proton-transfer reaction"
17:20-17:55 **Kiyoshi Yagi** (University of Yamanashi) "Vibrational theory for polyatomic molecules, clusters, and beyond"

WELCOME PARTY

February 22 (Mon.)

Session 3. Semiclassical Theory of Chemical Reactions and Non-adiabatic Processes

Chairperson: Koji Ando

9:00-9:35 **Ke-Li Han** (Dalian Institute of Chemical Physics) "The 3D nonadiabatic dynamics calculation of DH2+ and HD2+ systems by using the trajectory surface hopping method based on the Zhu-Nakamura theory"
9:35-10:10 **Alexey D. Kondorskiy** (P. N. Lebdev Physical Institute) "Semiclassical Wave Packet Propagation Method for Electronically Nonadiabatic Chemical Dynamics"

Chairperson: Katsuyuki Nobusada

10:30-11:05 **Laurent Bonnet** (Universite Bordeaux I) "Classical Reactive Scattering in a Quantum Spirit"
11:05-11:40 **Yi Zhao** (Xiamen University) "Approaches on electron transfer rate constants from weak-to-strong electronic coupling regimes"

Session 4. Laser Control of Chemical Dynamics

Chairperson: Tahei Tahara

13:10-13:45 **Hirohiko Kono** (Tohoku University) "Nonadiabatic response of molecules to time-dependent fields"
13:45-14:20 **Tsuyoshi Kato** (University of Tokyo) "Development of time-dependent multiconfiguration wave function theory for electronic and molecular dynamics in intense laser fields"
14:20-14:55 **Kenji Ohmori** (Institute for Molecular Science) "Spatiotemporal coherent control with picometer and attosecond precision; From cold molecules to bulk solids"

Chairperson: Alexey D. Kondorskiy

15:15-15:50 **Yukiyoshi Ohtsuki** (Tohoku University) "Development of optimal control simulation and its applications to molecular alignment and quantum information processing"
15:50-16:25 **Michihiko Sugawara** (Keio University)"A new control scheme for multi-level quantum system based on effective decomposition by intense CW-laser fields"

Session 5. Semiclassical dynamics and ab initio MD

Chairperson: Motoyuki Shiga

16:45-17:20 **Nikos Doltsinis** (King's College London) "Multiscale Modelling of Photoactive Materials"
17:20-17:55 **Shigehiko Hayashi** (Kyoto University) "Photochemical Reaction Dynamics of Retinal Proteins"
17:55-18:30 **Tetsuya Taketsugu** (Hokkaido University) "Ab initio molecular dynamics approach to excited-state reactions"

BANQUET (Okazaki New Grand Hotel)

February 23 (Tue.)

Session 6. Quantum Effects in Condensed Phases

Chairperson: Shinji Saito

9:00- 9:35 **Kenichi Kinugawa** (Nara Women's University) "Dynamics of condensed phase hydrogen explored by means of path integral centroid molecular dynamics simulations"
9:35-10:10 **Shinichi Miura** (Kanazawa University) "Molecular Dynamics Algorithms for Quantum Monte Carlo Methods"
10:10-10:45 **Motoyuki Shiga** (Japan Atomic Energy Agency) "Ab initio path integral simulations"

Chairperson: Takeshi Yamamoto

11:05-11:40 **Toshiyuki Takayanagi** (Saitama Univ.) "Nuclear quantum effects in helium complex and uracil anion"
11:40-12:15 **Koji Ando** (Kyoto University) "Semiquantal wavepacket modeling of reaction dynamics and chemical bonding"

Chairperson: Haruki Ishikawa

13:30-14:05 **Tahei Tahara** (RIKEN) "Coherent Nuclear Dynamics in Primary Ultrafast Chemical Processes"
14:05-14:40 **Atsushi Yamada** (Nagoya University) "Mixed Quantum-Classical Molecular Dynamics Simulation of Intramolecular Proton Transfer Reaction in Solution: One-Dimensional Quantization Model Study"

Session 7. Molecular Design and Control of Molecular Functions

Chairperson: Kiyoshi Yagi

15:00-15:35 **Takayuki Ebata** (Hiroshima University) "Laser spectroscopic study on encapsulation structure of functional molecules in supersonic jets"
15:35-16:10 **Tomokazu Yasuike** (Institute for Molecular Science) "Photoinduced coherent dynamics of adsorbates on metal surfaces: nuclear wave packet simulation with quasi-diabatic potential energy curves obtained by open-boundary cluster model"
16:10-16:45 **Shinkoh Nanbu** (Sophia University) "Hydrogen encapsulation using non-adiabatic tunneling"
16:45-16:50 Closing remarks (Toshimasa Ishida)