The 2\textsuperscript{nd} International Seminar of

Frontier of Energy Flow Dynamics in Atomistic and Electronic Scales

1\textsuperscript{st} December, 2009

Aoba-Memorial Hall at Aobayama-Campus,

Tohoku University, Sendai, Japan

Program

Sponsored by Global COE Program
“World Center of Education and Research for Trans-disciplinary Flow Dynamics”
Focus of FEFDAES-2

Energy flow phenomenon and their dynamics have been strenuously researched in many fields, such as display, semiconductor, catalyst, tribology and so on. Since the phenomena usually include many complexities, interaction and fusion between different fields are thus strongly needed to gain a further progress.

This seminar, entitled "Frontier of Energy Flow Dynamics in Atomistic and Electronic Scales (FEFDAES)", provides the frontier knowledge, especially for the energy flow dynamics in atomistic and electronic scales. The seminar invites some young researchers in the concerned fields and we will widely discuss the future direction of energy flow in atomistic and electronic scales.

All the presentations and discussions in FEFDAES-2 will be made by students. It could enhance the connections between students with a future. This aim corresponds to three topics in the agenda of education program of Tohoku University GCOE program:

- trans-disciplinary and broad perspective
- human network
- command of foreign languages

Organized and Sponsored by

The global COE program,

“World Center of Education and Research for Trans-disciplinary Flow Dynamics”

Organizing Committee

Chair
Hiroaki ONUMA
Ph. D. Student, Department of Applied Chemistry, Graduate School of Engineering, Tohoku University

Chair
Tasuku ONODERA
Ph. D. Student, Department of Applied Chemistry, Graduate School of Engineering, Tohoku University

Chair
Sunho JUNG
Ph. D. Student, Department of Chemical Engineering, Graduate School of Engineering, Tohoku University
Presentations

Oral presentation

- Invited talks (O-1 ~ O-6)
  Each invited speaker will be allowed to present in allotted 25 minutes (20 minutes for presentation, and 5 minutes for discussion).

- Short oral presentation (S-1 ~ S-18)
  Each invited speaker will be allowed to present in allotted 5 minutes (5 minutes for presentation, and no time for discussion).

- The official language is English.
- All oral presenters are required to bring their presentation data in a CD-R or USB memory stick, or their own laptop computer to PC operator desk located in the conference room.
- Speakers are required to scan their presentation data with the newest virus scan software prior to saving their data.
- Only LCD projection will be available. No overhead projector for transparencies will be available.
- The computers provided in the meeting rooms will be equipped with Microsoft Windows XP and Power Point 2003. For Apple Macintosh users: Please use your own computer.
- Speaker’s laptop computers must be equipped with a D-Sub 15 pin output, standard monitor terminal. Please bring an adapter for interface conversion if necessary.
- Speakers must operate the equipment during presentation, using the mouse and monitor at the podium.

Poster presentation

- All the speakers, including invited persons, must present own study in the poster session.
- The official language is English.
- All presenters must put up their posters on the designated boards between 10:00 and 16:45.
- After the poster session is closed, posters must be taken away by the presenters until 17:05. Posters left on the boards until 20:00 will be discarded.
- The schedule on the day of poster presentation is as follows:
  
  Mounting  09:30-10:30
  Presentation  15:45-16:45
  Removal  16:45-17:05

Boards and pushpins for poster setup will be provided. Each board size is 1200 mm (W) × 1740 mm (H). Posters should be placed within the area of the board. A0 size (841 mm × 1189 mm) may be appropriate, if the presenter wishes to prepare his/her poster as a single sheet.
# Program

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>09:30-</td>
<td>Registration</td>
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<tr>
<td>10:30-10:40</td>
<td>Opening remarks, welcome talk</td>
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<tr>
<td>10:40-11:05</td>
<td>Invited talk (O-1)</td>
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<td></td>
<td>Mr. Bart Trzynadlowski (University of Washington, USA)</td>
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<td></td>
<td><em>Tracking Extended Defects with a Stress-Dependent Reduced Kinetic Precipitation Model</em></td>
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<td>11:05-11:30</td>
<td>Invited talk (O-2)</td>
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<td>Mr. Sung Wook Kim (Korea Advanced Institute of Science and Technology, The Republic of Korea)</td>
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<td><em>Study of Excitation Energy Transfer in Fluorine Based Host-Guest Systems</em></td>
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<td>Mr. Ryo Kunimoto (Kyoto University, Japan)</td>
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<td><em>Prediction of MicroRNA-regulated Transcriptome Network</em></td>
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<td>Mr. Haruki Koda (Osaka University, Japan)</td>
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<td></td>
<td><em>Introduction to User Interface for Design Support</em></td>
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<tr>
<td>13:45-15:25</td>
<td>Short oral presentation (S-1 ~ S-18)</td>
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<td>15:25-15:45</td>
<td>Coffee break</td>
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<tr>
<td>15:45-16:45</td>
<td>Poster presentation (1st floor, all presenters)</td>
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<td>16:45-17:05</td>
<td>Poster removal</td>
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<td>17:05-17:30</td>
<td>Invited talk (O-5)</td>
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<td>Ms. Paule Njiwa (Ecole Centrale de Lyon, France)</td>
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<td><em>Tribology Behavior Composition of Two Anti-Wear Additives: Zinc Dialkyldithiophosphates (ZDDP) and Phosphate Dialky (ZP)</em></td>
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<td>17:30-17:55</td>
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<td>Mr. Hyoung Sun Yoo (Korea Advanced Institute of Science and Technology, The Republic of Korea)</td>
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<td><em>Fabrication of Phosphor Photonic Crystal by Self-assembly of Monodisperse Spherical Phosphor Particles</em></td>
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<td>17:55-</td>
<td>Closing remarks</td>
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<td>18:15-20:00</td>
<td>Banquet (3rd floor, “四季彩—SHIKISAI”)</td>
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Oral presentation

O-1 Invited Tracking Extended Defects with a Stress-Dependent Reduced Kinetic Precipitation Model
Mr. Bart Trzynadlowski
University of Washington, USA
(10:40-11:05)

O-2 Invited Study of Excitation Energy Transfer in Fluorine Based Host-Guest Systems
Mr. Sung Wook Kim
Korea Advanced Institute of Science and Technology, The Republic of Korea
(11:05-11:30)

O-3 Invited Prediction of MicroRNA-regulated Transcriptome Network
Mr. Ryo Kunimoto
Kyoto University, Japan
(11:30-11:55)

O-4 Invited Introduction to User Interface for Design Support
Mr. Haruki Koda
Osaka University, Japan
(13:20-13:45)

O-5 Invited Tribology Behavior Composition of Two Anti-Wear Additives: Zinc Dialkyldithiophosphates (ZDDP) and Phosphate Dialkyl (ZP)
Ms. Paule Njiwa
Ecole Centrale de Lyon, France
(17:05-17:30)

O-6 Invited Fabrication of Phosphor Photonic Crystal by Self-assembly of Monodisperse Spherical Phosphor Particles
Mr. Hyoung Sun Yoo
Korea Advanced Institute of Science and Technology, The Republic of Korea
(17:30-17:55)
Short oral presentation

S-1  Influence of the Surface Hydrogen Vacancy for the Dissociative Adsorption of H\textsubscript{2} on Pd (111) Surface: A Molecular Dynamics Study
Mr. Farouq Ahmed, Tohoku University, Japan

S-2  Estimation of Secondary Electron Emission Coefficient: Computational Study for Improving Energy Flow in PDP
Mr. Kazumi Serizawa, Tohoku University, Japan

S-3  Analyzing Electrochemical Properties of Cation-doped LiFePO\textsubscript{4} Using a Tight-Binding QCMD Calculation
Ms. Tomomi Shimo, Tohoku University, Japan

S-4  A Computational Study on the Automotive Catalytic Reaction
Mr. Sunho Jung, Tohoku University, Japan

S-5  Invited Preparation and NO Reduction Property of Apatite-type Silicate Supported Pt Catalyst
Mr. Atsunori Ono, Akita University, Japan

S-6  Study on p53 Inactivation Mechanism by Viral Oncoprotein LTag, an UA-QCMD approach
Mr. Shah Md. Abdul Rauf, Tohoku University, Japan

S-7  Computational Chemistry Study on Electrode Characteristic of PEFC
Mr. Hiroshi Kobayashi, Tohoku University, Japan

S-8  Theoretical Investigation of Fucosylated Oligosaccharide Fragmentation by Using Quantum Chemical Molecular Dynamics Method
Ms. Xiaolei Wang, Tohoku University, Japan

S-9  A Large Scale Quantum Chemistry Calculation on Degradation of Blue Light-Emitting Polymer
Mr. Itaru Yamashita, Tohoku University, Japan

S-10 Advanced Quantum Chemical Molecular Dynamics Study to Investigate Interactions of Anti-HIV Drug with Target Protein
Mr. Kamlesh Kumar Sahu, Tohoku University, Japan
S-11  Computational Chemistry and Experimental Investigations on Boundary Friction of Fullerene Thin Film  
Mr. Tasuku Onodera, Tohoku University, Japan

S-12  A Study on the Cathode Catalyst Layer Degradation in PEFC Using Computational Chemistry Method  
Mr. Donghyun Kim, Tohoku University, Japan

S-13  A Multi-Scale Simulation on Dye-Sensitized Solar Cells with Metal-Free Organic Dye  
Ms. Mari Onodera, Tohoku University, Japan

S-14  Dynamic Behavior of Polarization Using TBQCMD  
Mr. Kenji Kondou, Tohoku University, Japan

S-15  Reaction Mechanisms of CeO$_2$ (111) and CeO$_2$ (110) by H$_2$: A Quantum Chemical Molecular Dynamics Study  
Mr. Khorshed Md. Alam, Tohoku University, Japan

S-16  A Theoretical Study on Excited Energy Distributions in Inorganic Phosphor Crystals  
Mr. Hiroaki Onuma, Tohoku University, Japan

S-17  Electronic Structure Analysis of Transparent Electrode Material Using Tight-Binding Quantum Chemistry Calculation  
Mr. Sho Hirose, Tohoku University, Japan

S-18  Initial Oxidation Stages of the 4H-SiC(0001) Surface and its Interface with SiO$_2$: A Quantum Chemical Molecular Dynamics Study  
Mr. John Poul Yacapin, Tohoku University, Japan