



# 7<sup>th</sup> International Symposium on Molecular Thermodynamics and Molecular Simulation (MTMS'15)

Fukuoka University, Fukuoka, Japan August 4-7, 2015

<http://mtms15.jimdo.com/>



## Scope

The 7<sup>th</sup> International Symposium on “Molecular Thermodynamics and Molecular Simulation (MTMS'15)” will be held during August 4-7, 2015 at Nanakuma Campus of Fukuoka University in Fukuoka, Japan. The objective of this four-day symposium is to provide a forum for scientists and engineers to discuss the recent advances in fluid properties and their theoretical description. The symposium is structured with a single plenary lecture, several keynote lectures by eminent scientists and engineers, invited lectures on selected topics and oral and poster presentations. MTMS was established in 1994 by the *late* Professor Koichiro Nakanishi. MTMS has been held and organized at three-year intervals since 1994 :

## Topics

- Molecular thermodynamics
- Molecular simulations and techniques
- Process design
- Equation of state
- Solution structure
- Supercritical fluids
- Macromolecules
- Thermophysical properties
- Quantum simulations
- Process simulation
- Activity coefficient
- Mesoscopic systems
- Ionic liquids
- Polymers

## Important dates

Abstract deadline for orals and posters	April 15, 2015
Early registration	April 1 - June 30, 2015
Letter of acceptance from committee	April 30, 2015
Deadline for proceedings submission	<b>June 30, 2015</b>
<b>MTMS'15 Symposium</b>	<b>August 4-7, 2015</b>

## Registration

Registration fee

	General	Student
before June 30, 2015	50,000JPY	25,000JPY
after June 30, 2015	55,000JPY	30,000JPY

Additional fees for conference dinner and conference banquet

	General	Student
Dinner on Aug. 5 (Wed)	5,000JPY	4,000JPY
Banquet on Aug. 6 (Thur)	10,000JPY	8,000JPY

## Tentative Program\*

Tuesday, August 4	17:00-20:00 Registration at Fukuoka Toei Hotel 18:00-20:00 Welcome reception at Fukuoka Toei Hotel
Wednesday, August 5	8:30-12:00, 14:00-19:00 Registration at Fukuoka Univ. 8:30-19:00 Opening, Plenary and Keynote lectures, Oral presentations at Fukuoka Univ. (12:30-13:30 Lunch time) 19:00- Dinner at Fukuoka Univ.
Thursday, August 6	8:30-12:00 Registration at Fukuoka Univ. 8:30-12:30 Oral and poster presentations at Fukuoka Univ. (12:30-13:30 Lunch time) 13:30- Excursion (Karatsu Castle etc.) 19:00- Banquet at Marizon
Friday, August 7	8:30-12:00 Registration at Fukuoka Univ. 8:30- 13:30 Oral presentations, Closing at Fukuoka Univ. (12:30-13:30 Lunch time)

\*Additional information will be announced on the web site:

<http://mtms15.jimdo.com/>

# Outline of scientific program

## Plenary speaker

- Prof. Clare McCabe (Vanderbilt Univ., USA)

## Keynote speakers

- Prof. Peter Cummings (Vanderbilt Univ., USA)

- Prof. Jeong Won Kang (Korea Univ., Korea)

New modified UNIFAC parameters using critically evaluated phase equilibrium data

- Prof. Georgios M. Kontogeorgis (Tech. Univ. Denmark, Denmark)

Equations of state in three centuries – Perspectives and future challenges

- Prof. José Nuno Canongia Lopes (Instituto Superior Técnico, Portugal)

Probing the distinctive interactions and structures of ionic liquids and their mixtures using MD simulations and different aggregation analysis tools

- Prof. Cor J. Peters (Petro. Ins., UAE)

Ionic liquids versus deep eutectic solvents

## Invited speakers

- Dr. Nevin Gerek Ince (Schneider Electric, USA)

PC-SAFT equation of state: Application to polymer systems in dynamic simulation suite (DynSim) by Schneider Electric

- Prof. Kwak Sang Kyu (UNIST, Korea)

Prediction of phase transition of FCC and HCP hard-sphere crystals via Free Volume Approach

- Prof. Zhiping Liu (Beijing Univ. Chem. Tech., China)

Infinite dilute activity coefficients and liquid-liquid equilibria of binary systems containing ionic liquids predicted by COSMO-RS method

- Prof. Gabrielle Sadowski (TU Dortmund, Germany)

Solvent influence on esterification equilibria

- Prof. Md. Zaidul Islam Sarker (Int. Islamic Univ., Malaysia)

Green process for producing nutraceutical oils from tropical plants - unused seeds of Mahkota Dewa (*Phaleria macrocarpa*) fruit.

- Prof. Jae-Jin Shim (Yeungnam Univ., Korea)

Controlled living polymerization in supercritical carbon dioxide

- Dr. Seiji Tsuzuki (AIST, Japan)

Relationship between interionic interaction and transport properties of ionic liquids: Analysis by ab initio MO calculations and MD simulations

- Prof. Wenchuan Wang (Beijing Univ. Chem. Tech., China)

Multiscale modeling and preparations of nano-porous materials: H<sub>2</sub> storage and CO<sub>2</sub> capture

- Prof. Suojiang Zhang (Inst. Proc. Eng. Chinese Acad. Sci., China)

Z-bond and molecular simulation of ionic liquids

## The other contributions

### 13 Oral and 50 Poster presentations

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## Committees

### Executive committee:

#### Chair:

- Yoshio Iwai (Kyushu Univ., Japan)

#### Co-Chair:

- Kenji Mishima (Fukuoka Univ., Japan)
- Kiyofumi Kurihara (Nihon Univ., Japan)
- Shigeo Oba (App. Thermody. Phys. Prop. Co., Japan)

### Advisory committee:

- Yasuhiko Arai (Japan)
- Hirokatsu Masuoka (Japan)
- Hideo Nishiumi (Japan)
- Shuzo Ohe (Japan)
- Katsumi Tochigi (Japan)

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- Peter Cummings (Vanderbilt Univ., USA)
- Nevin Gereck Ince (Schneider Electric, USA)
- Jeong Won Kang (Korea Univ., Korea)
- Georgios M. Kontogeorgis (Tech. Univ. Denmark, Denmark)

- Kwak Sang Kyu (UNIST, Korea)

- Zhiping Liu (Beijing Univ. Chem. Tech., China)

- José Nuno Canongia Lopes (Instituto Superior Técnico, Portugal)

- Clare McCabe (Vanderbilt Univ., USA)

- Cor J. Peters (Petro. Ins., UAE)

- Gabrielle Sadowski (TU Dortmund, Germany)

- Md. Zaidul Islam Sarker (Int. Islamic Univ., Malaysia)

- Jae-Jin Shim (Yeungnam Univ., Korea)

- Wenchuan Wang (Beijing Univ. Chem. Tech., China)

- Suojiang Zhang (Inst. Proc. Eng. Chinese Acad. Sci., China)

### Organizing Committee:

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- Hirohisa Uchida (Shinshu Univ., Japan)

- Morio Yamamoto (Sumitomo Chem. Co., Japan)

### Scientific Secretary:

- Setsuko Yonezawa (Kyushu Univ., Japan)

E-mail: syone@chem-eng.kyushu-u.ac.jp