



MTMS '18

8th International Symposium on
Molecular **T**hermodynamics and
Molecular **S**imulation

Program Book



September 4-7, 2018

Tsudanuma Campus of Nihon University,
Narashino, Japan



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Preface

The objective of “Molecular Thermodynamics and Molecular Simulation (MTMS)” is to provide a forum for scientists and engineers to discuss the recent advances in fluid properties and their theoretical description. MTMS was established in 1994 by the late Professor Koichiro Nakanishi. MTMS has been held and organized at three-year intervals since 1994:

	Date	Venue	Chair/Organizer
1 st	1994	Kyoto	-Prof. Koichiro Nakanishi (Kyoto Univ.)
2 nd	1997	Tokyo	-Prof. Hideo Nishiumi (Hosei Univ.)
3 rd	2003	Sendai	-Prof. Hiroshi Inomata (Tohoku Univ.)
4 th	2006	Makuhari	-Prof. Toshihiko Hiaki (Nihon Univ.)
5 th	2009	Kanazawa	-Prof. Kazuhiro Tamura (Kanazawa Univ.)
6 th	2012	Higashi-Hiroshima	-Prof. Shigeki Takishima (Hiroshima Univ.)
7 th	2015	Fukuoka	-Prof. Yoshio Iwai (Kyushu Univ.)

The 8th International Symposium on “Molecular Thermodynamics and Molecular Simulation (MTMS’18)” is held during September 4-7, 2018 at Tsudanuma Campus of Nihon University in Narashino, Japan. The symposium is organized by Division of Physical Properties, the Society of Chemical Engineers, Japan and Division of Supercritical Fluids, the Society of Chemical Engineers, Japan. We want to discuss not only the fluid properties but also the applications of fluid properties at the symposium. The symposium is structured with one plenary lecture, 5 keynote lectures by eminent scientists and engineers, 7 invited lectures on selected topics, 19 oral presentations, and 67 poster presentations.

Narashino city is located in Chiba, East Japan, bordered by Tokyo Bay to the southwest. It’s easily accessible from not only Narita and Haneda airports but also sightseeing spots in Tokyo. Also, it has a lot of nature. Especially Yatsu-higata, which registered in the Ramsar Convention, is very famous tidal flat for birds’ oasis. We will make an excursion to Naritasan Shinshoji Temple in Chiba. This time-honored temple has a history of over 1000 years, during which it has attracted many believers. We hope all the participants enjoy Japanese Buddhism, cultures, and history.

On behalf of the organizing committee, I would like to thank all the authors for their contribution and also thank all the participants for their kind interest given to the symposium. I appreciate all the sponsors for their financial supports.

I hope all the participants will enjoy the symposium and Narashino City.

Kiyofumi Kurihara
Symposium Chair

MTMS ’18, Narashino, Japan, September 4 – 7, 2018



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Timetable

September 4, 2018 (Tuesday)

17:00 – 20:00	Registration at Gallery on 1st floor
18:00 – 20:00	Welcome Reception at Cafeteria "Creation Commons" on 2nd floor

September 5, 2018 (Wednesday)

8:00 – 18:00	Registration at Gallery on 1st floor
8:30 – 8:40	Opening Remarks
8:40 – 9:20	Plenary Lecture
9:20 – 10:30	Session I
10:30 – 10:50	Coffee Break
10:50 – 12:40	Session II
12:40 – 13:50	Lunch at Cafeteria "Creation Commons" on 2nd floor
13:50 – 15:40	Session III
15:40 – 16:00	Coffee Break
16:00 – 18:00	Session IV
18:00 – 20:00	Dinner at Cafeteria "Creation Commons" on 2nd floor

September 6, 2018 (Thursday)

8:00 – 12:20	Registration at Gallery on 1st floor
8:30 – 9:00	Session V
9:00 – 10:00	Session VI Flash Presentation for Young Researchers
10:00 – 12:20	Poster Session at Gallery on 1st floor
12:20 – 13:40	Lunch at Cafeteria "Creation Commons" on 2nd floor
13:40 – 13:50	Group Photo
13:50 – 19:00	Excursion at Naritasan Shinshoji Temple
19:00 – 21:00	Banquet at Sapporo Breweries Chiba Beer Restaurant

September 7, 2018 (Friday)

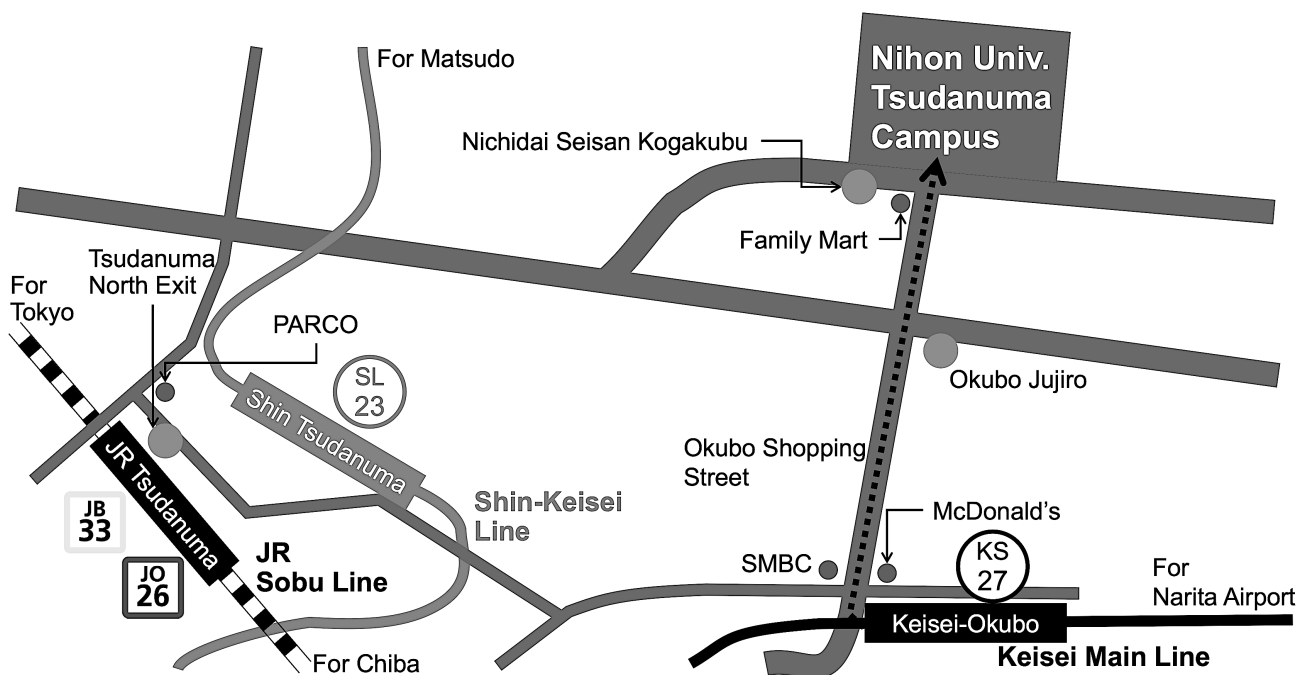
8:00 – 12:00	Registration at Gallery on 1st floor
8:30 – 10:40	Session VII
10:40 – 11:00	Coffee Break
11:00 – 13:00	Session VIII
13:00 – 13:10	Closing Remarks and Student Poster Award



General Information

Access Information

1. Access Map to Conference Venue: Tsudanuma campus of Nihon University



By Walk: A 10-minute walk from the exit of Keisei Okubo Station on the Keisei Main Line.

By Bus: Take the bus from the No. 4 or No. 5 bus stop at the north exit of JR Tsudanuma Station to the “Nichidai Seisan Kogakubu” bus stop.

NOTE: From the conference venue, take the bus from the “Okubo Jujiro” bus stop.

2. Campus Map of Tsudanuma campus of Nihon University

Venue is Building 39 on Tsudanuma campus of Nihon University, except Excursion and Banquet on September 6.



Registration Desk Gallery on first floor

Welcome Reception on September 4 and Conference Dinner on September 5

Cafeteria "Creation Commons" on second floor

Presentations Oral: Room 308 on third floor Poster: Gallery on first floor

Cloak third floor

Lunch Cafeteria "Creation Commons" on second floor

Smoking Area Between conference place (Building 39) and Building 25. Please see "Smoking Area".

3. Access to Banquet on September 6, 19:00- Sapporo Breweries Chiba Beer Restaurant

NOTE: After excursion, bus takes you banquet place. Please check the following URL if you directly go to the banquet place.

2 Takasemachi Funabashi-shi, Chiba, 273-0014

URL (Japanese): <http://r.gnavi.co.jp/g175401/>

Free shuttle bus from JR Tsudanuma, JR Shin-Narashino, and JR Minami-Funabashi stations (Japanese):
http://www.sapporobeer.jp/brewery/chiba/access/chiba_jikoku2.html

Registration Desk

Registration desk is located at the gallery on the first floor in Building 39. It will be open:

Tuesday, September 4 – from 17:00 to 20:00

Wednesday, September 5 – from 8:00 to 18:00

Thursday, September 6 – from 8:00 to 12:20

Friday, September 7 – from 8:00 to 12:00

Certificate of Attendance and Receipt

Certificate of attendance and receipt can be found in your bag which will be handed at the registration desk.

Cloak

Cloak service can be available on the third floor in Building 39. It will be open:

Wednesday, September 5 – from 8:00 to 20:00

Thursday, September 6 – from 8:00 to 13:30

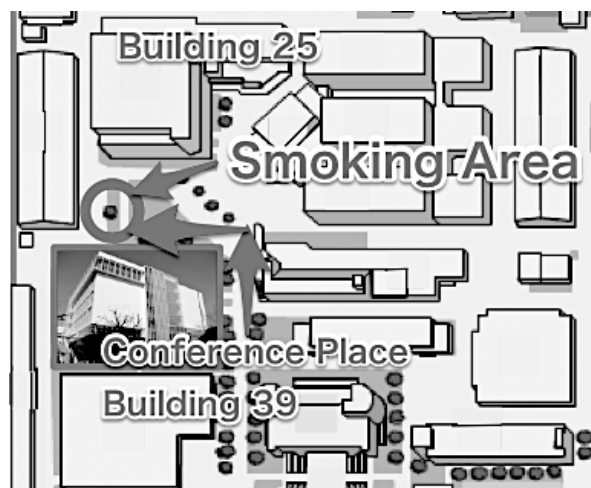
Friday, September 7 – from 8:00 to 13:30

Wi-Fi

Wi-Fi service will be available across the conference room. Instructions will be announced during the conference.

Smoking Area

Smoking area in this campus is located between the conference place (Building 39) and Building 25. This



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campus is non-smoking except the smoking area.

Lunch and Coffee

Lunch will be served on September 5 and 6. It will be organized Japanese Bento box style in Cafeteria "Creation Commons" on the second floor. Coffee will be served on the third floor on September 5 and 7, or at the gallery on the first floor on September 6. **Please note that lunch on September 7 will not be served.**

Group Photo

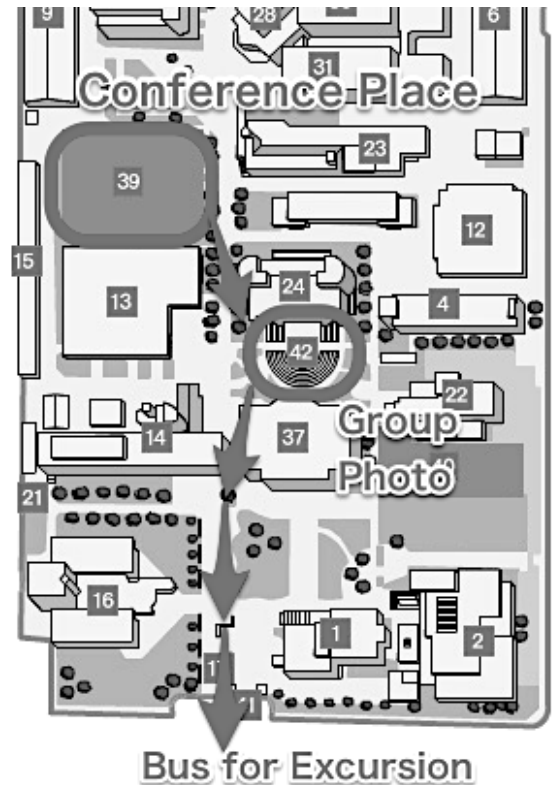
Group photo of the participants will be taken at 13:40 on September 6 in "Sunken Plaza" near Building 24.

Excursion

Naritasan Shinshoji Temple

Naritasan Shinshoji temple is a time-honored temple with a history of over 1000 years since its foundation. It is a temple complex with many different temple buildings and a park. You can enjoy experience a touch of Japanese history first hand.

URL: <http://www.naritasan.or.jp/english/>



NOTE:

- **Bus for excursion departs at 13:50 on September 6, after group photo.**
- **After excursion, bus takes you to banquet place.**

Banquet on September 6, 19:00-

Banquet is held in Sapporo Breweries Chiba Beer Restaurant. It is located in Tokyo Bay area. You can enjoy fresh beer and barbecue, while enjoying the ocean view. After the banquet, bus will take you to JR Tsudanuma, JR Minami-Funabashi, or Keisei Tsudanuma stations.

Clothes

We recommend “cool biz” clothes. “Cool biz” is a term made up from the words “cool” and “biz” (an abbreviation for business). We are recommended to reduce to use air conditioners in offices for energy saving and carbon dioxide emission reduction. However, the temperature and humidity will be very high in Chiba during the conference. The solution is “cool biz”. **We strongly recommend all the participants to remove your ties and jackets during the conference.**

Also, banquet on September 6 does not have any dress code, since it is held after excursion of Naritasan Shinshoji Temple. Please enjoy excursion and banquet with casual clothes.

Student Poster Presentation Award

Student poster presentation award is given for the students who make excellent poster presentation. Invited lectures will be a referee. Award ceremony will be held in the closing remarks on September 7.

Special Issue

The organizing committee is pleased to announce a special issue of the Elsevier journal Fluid Phase Equilibria for papers presented at MTMS '18. Detailed information will be announced during the conference.

Instructions for Presenter

1. Oral Presentation (Plenary, Keynote, Invited, or Oral)

- Authors should prepare oral presentations with a total duration of 40 minutes (plenary and keynote lectures), 30 minutes (invited lectures), or 20 minutes (oral presentations) including questions (approx. 4 or 5 minutes per talk).
- A projector with VGA connector will be available. Presenters must bring their own laptop for computer presentations. In preparation for the unexpected, please also have your presentation data by USB flash drive. In addition, if you are a Mac user, you will need to bring a VGA adapter.
- We will prepare a laptop (Windows) with Power Point as a backup.



VGA Connector

2. Flash Presentation for Young Researchers

- Flash presentation for young researchers is held in the morning on September 6.
- This session has five oral presentations in the tentative program.
- Authors should prepare oral presentations with 10 minutes.
- Time of questions for five presenters will be 10 minutes.
- We prepare a laptop (Windows) with Power Point. Please have your presentation data by USB flash drive.
- Please contact staff in Room 308 (3rd floor of conference building) until 8:30 AM on September 6, in order to upload your presentation data from your USB flash drive.

3. Poster Presentation

- Poster session is held in the morning on September 6.
- Please prepare your poster so that it fits within 90 cm in width and 170 cm in height.
- You can put up your poster on the board from September 5.
- Poster number (PP **) is in the left side of the board.
- Pins to put up your poster will be available in the poster place.
- Please remove your poster immediately after the poster session.



Technical Program

September 5, 2018 (Wednesday)

8:30 – 8:40	Opening Remarks Prof. Kiyofumi Kurihara (Nihon University, Japan)
8:40 – 9:20	Plenary Lecture PL 01 Chair: Prof. Yoshio Iwai (Kyushu University, Japan)
	Molecular design and prediction of structure and physical properties of complex chemical systems of importance to the oil and gas industry Ioannis G. Economou* Texas A&M University at Qatar, Qatar
9:20 – 10:30	Session I Chair: Dr. Z. Nevin Gerek (AVEVA Group plc., USA) and Prof. Katsumi Tochigi (Nihon University, Japan)
9:20 – 10:00	Keynote Lecture KL 01 Examining the self-assembly of stratum corneum lipid mixtures Tim Moore, Donna Xia, Anne Leonhard, Chris Iacovella, <u>Clare McCabe</u> * Vanderbilt University, USA
10:00 – 10:30	Invited Lecture IL 01 Correlation of phase equilibria by new activity coefficient model <u>Yoshio Iwai</u> *, Ryosuke Seki, Yoshihiro Tanaka Kyushu University, Japan
10:30 – 10:50	Coffee Break
10:50 – 12:40	Session II Chair: Prof. Richard L. Smith (Tohoku University, Japan) and Prof. Tetsuo Honma (National Institute of Technology, Hachinohe College, Japan)
10:50 – 11:30	Keynote Lecture KL 02 Computational screening of soft materials systems with application to nano-lubrication systems Andrew Z. Summers, Christopher R. Iacovella, Clare McCabe, <u>Peter T. Cummings</u> * Vanderbilt University, USA
11:30 – 12:00	Invited Lecture IL 02 Multiscale modeling and simulations of protein adsorption at interfaces Jian Zhou* South China University of Technology, P. R. China
12:00 – 12:20	OP 01 Numerical simulation for the motion of a single bubble on the vertical wall surface by a lattice Boltzmann method for two-phase flow with large density difference <u>Tomohiko Yamaguchi</u> *, Satoru Momoki Nagasaki University, Japan

12:20 – 12:40	OP 02
Thermodynamic modeling of adsorption equilibria of metal precursors on mesoporous silica adsorbents in supercritical carbon dioxide with SAFT-VR approach	
<u>Ikuo Ushiki</u> ^{*1} , Mio Koike ² , Yoshiyuki Sato ² , Shigeki Takishima ¹ , Hiroshi Inomata ²	
¹ Hiroshima University, Japan ² Tohoku University, Japan	
12:40 – 13:50	Lunch
13:50 – 15:40	Session III
Chair: Prof. Edward Maginn (University of Notre Dame) and Prof. Taka-aki Hoshina (Nihon University, Japan)	
13:50 – 14:30	Keynote Lecture KL 03
Current status and challenges in electrolyte thermodynamics	
Georgios M. Kontogeorgis [*]	
Technical University of Denmark, Denmark	
14:30 – 15:00	Invited Lecture IL 03
Molecular dynamics simulation study on the correlations between macroscopic properties and microscopic interactions of CO₂ physical absorbents	
Ryo Nagumo [*]	
Nagoya Institute of Technology, Japan	
15:00 – 15:20	OP 03
Effective charge of ionic liquid determined through MD/DFT self-consistent scheme	
<u>Ryosuke Ishizuka</u> ^{*1,2} , Nobuyuki Matubayasi ^{1,2}	
¹ Osaka University, Japan ² Kyoto University, Japan	
15:20 – 15:40	OP 04
Measurement of diffusion coefficients of vitamin K₃ in mixture of CO₂ and methanol over an entire range of methanol at 313.2 K up to 30 MPa	
Ryusei Suzuki ¹ , Junichi Sakabe ¹ , <u>Toshitaka Funazukuri</u> ^{*1} , Chang Yi Kong ²	
¹ Chuo University, Japan ² Shizuoka University, Japan	
15:40 – 16:00	Coffee Break
16:00 – 18:00	Session IV
Chair: Prof. Takeshi Momose (University Tokyo, Japan) and Dr. Mitsuhiro Kanakubo (AIST, Japan)	
16:00 – 16:40	Keynote Lecture KL 04
Using reaction ensemble Monte Carlo simulations to understand how solvation and confinement affects equilibrium concentrations of reacting mixtures	
Ryan Gotchy Mullen, <u>Edward J. Maginn</u> [*]	
University of Notre Dame, USA	
16:40 – 17:00	OP 05
Preparation of solid acid catalysts from seaweed for the esterification of biomass-based components	

Mitsuru Sasaki^{*,1}, Shamala Balasubramaniam¹, Shohei Ninomiya¹, Armando T. Quitain¹, Tetsuya Kida¹, Marleny Aranda Saldana²

¹ Kumamoto University, Japan ² University of Alberta, Canada

17:00 – 17:20 OP 06

Phase behavior and reactivity of ionic liquid catalysts for esterification of long-chain fatty alcohols/carboxylic acids under mild conditions

Yuki Kohno^{*}, Takashi Makino, Mitsuhiro Kanakubo

National Institute of Advanced Industrial Science and Technology (AIST), Japan

17:20 – 17:40 OP 07

The extraction of the receptacle and leaf of strawberry with supercritical carbon dioxide and entrainers

Takafumi Sato^{*}, Fumika Fukuda, Yoshiro Ikeya, Ken-ichi Nihei, Naotsugu Itoh

Utsunomiya University, Japan

17:40 – 18:00 OP 08

Measurement of vapor pressure of various compounds by gas chromatographic method with mass-basis activity coefficient

Jun Mase^{1,2}, Yusuke Shimoyama^{*,2}

¹ Idemitsu Kosan Co., Ltd., Japan

² Tokyo Institute of Technology, Japan

18:00 – 20:00

Dinner

September 6, 2018 (Thursday)

8:30 – 9:00	Session V
Chair: Prof. Takeshi Sugahara (Osaka University, Japan) and Dr. Seiya Hirohama (AVEVA Group plc., USA)	
8:30 – 9:00	Invited Lecture IL 04
Challenges and solutions for next generation process simulators	
Z. <u>Nevin Gerek Ince</u> [*] , Seiya Hirohama, David Bluck	
AVEVA Group plc., USA	
9:00 – 10:00	Session VI Flash Presentation for Young Researchers
Chair: Prof. Takeshi Sugahara (Osaka University, Japan) and Dr. Seiya Hirohama (AVEVA Group plc., USA)	
9:00 – 9:10	FP 01
Phase behavior and phase equilibria for the polydisperse polyethylene + ethylene + hexane system at high pressures and temperature: Experiments and Correlations	
<u>Rizqy Romadhona Ginting</u> , Daichi Nakata, Kazunori Himemura, Ikuo Ushiki, Shin-ichi Kihara, Shigeki Takishima [*]	
Hiroshima University, Japan	
9:10 – 9:20	FP 02
Measurement of binary diffusion coefficient for Cr(acac)₃ in high temperature region of supercritical carbon dioxide	
<u>Minoru Yamamoto</u> ¹ , Sakabe Junichi ¹ , Toshitaka Funazukuri ^{*,1} , Chang Yi Kong ²	
¹ Chuo University, Japan ² Shizuoka University, Japan	
9:20 – 9:30	FP 03
Increased biocatalytic activity in CO₂-expanded bio-based liquids	
<u>Hai Nam Hoang</u> ¹ , Emanuel Granero-Fernandez ² , Shinjiro Yamada ¹ , Shuichi Mori ³ , Hiroyuki Kagechika ³ , Yaocihuatl Medina-Gonzalez ² , Tomoko Matsuda ^{*,1}	
¹ Tokyo Institute of Technology, Japan ² Université de Toulouse, France	
³ Tokyo Medical and Dental University, Japan	
9:30 – 9:40	FP 04
Density, viscosity, and CO₂/CH₄ solubility selectivity in protic and aprotic ionic liquids	
<u>Masaki Watanabe</u> ¹ , Daisuke Kodama ^{*,1} , Takashi Makino ² , Mitsuhiro Kanakubo ²	
¹ Nihon University, Japan	
² National Institute of Advanced Industrial Science and Technology (AIST), Japan	
9:40 – 9:50	FP 05
Thermodynamic property measurements and modeling for chemical hydrogen storage mediums	

Seishin Sato¹, Yuya Yoneda¹, Hiroyuki Miyamoto^{*,1}, Ryo Akasaka², Eric W. Lemmon³

¹ Toyama Prefectural University, Japan

² Kyusyu Sangyo University, Japan

³ National Institute of Standards and Technology (NIST), USA

9:50 – 10:00	FP 01 – FP 05 Discussion
10:00 – 12:20	Poster Session
12:20 – 13:40	Lunch
13:40 – 13:50	Group Photo
13:50 – 19:00	Excursion
19:00 – 21:00	Banquet

September 7, 2018 (Friday)

8:30 – 10:40	Session VII
Chair: Prof. Daisuke Kodama (Nihon University, Japan) and Prof. Mitsuru Sasaki (Kumamoto University, Japan)	
8:30 – 9:10	Keynote Lecture KL 05
Capturing impurities from oil and gas using deep eutectic solvents	
Samah E.E Warrag ^{1,2} , Cor J. Peters ^{*,1,3}	
¹ Khalifa University of Science and Technology, United Arab Emirates	
² Eindhoven University of Technology, The Netherlands ³ Colorado School of Mines, USA	
9:10 – 9:40	Invited Lecture IL 05
Generation of pulsed arc discharge plasma in supercritical carbon dioxide	
Tomohiro Furusato ^{*,1} , Naokazu Ashizuka ¹ , Kosuke Goto ¹ , Takahiko Yamashita ¹ , Tetsuo Honma ² , Mitsuru Sasaki ³	
¹ Nagasaki University, Japan ² National Institute of Technology, Hachinohe College, Japan	
³ Kumamoto University, Japan	
9:40 – 10:00	OP 09
CO₂ solubility and phase behavior in phase separation solvent at high pressure	
Andrzej-Alexander Litwinowicz ¹ , Takashi Makino ¹ , Yuki Kohno ¹ , Hiroshi Machida ² , Koyo Norinaga ² , Mitsuhiro Kanakubo ^{*,1}	
¹ National Institute of Advanced Industrial Science and Technology, Japan	
² Nagoya University, Japan	
10:00 – 10:20	OP 10
Solubility prediction of CO₂ in ionic liquids	
Hideo Nishiumi [*]	
Hosei University, Japan	
10:20 – 10:40	OP 11
Structure II hydrate formation with amine toward new gas separation process	
Sanehiro Muromachi ^{*,1,2} , Hassan Sharifi ¹ , John A. Ripmeester ^{1,3} , Peter Englezos ¹	
¹ The University of British Columbia, Canada	
² National Institute of Advanced Industrial Science and Technology (AIST), Japan	
³ National Research Council of Canada, Canada	
10:40 – 11:00	Coffee Break
11:00 – 13:00	Session VIII
Chair: Prof. Ikuo Ushiki (Hiroshima University, Japan) and Dr. Takashi Makino (AIST, Japan)	
11:00 – 11:30	Invited Lecture IL 06
Development of fast continuous supercritical CO₂ extraction/separation process using micromixer	
Tatsuya Fujii ^{*,1} , Yasuaki Matsuo ¹ , Shin-ichiro Kawasaki ¹	

¹ National Institute of Advanced Industrial Science and Technology (AIST), Japan.

11:30 – 12:00 Invited Lecture IL 07

Materials informatics for designing functional liquids

Hirotooshi Mori*

Ochanomizu University, Japan

12:00 – 12:20 OP 12

Development of simulation technology for cement manufacturing process

Morihisa Yokota*, Taturou Izumi, Takeshi Suemasu

UBE Industries, Ltd., Japan

12:20 – 12:40 OP 13

A prediction method of vapor pressure from boiling point data

Shuzo Ohe*

Tokyo University of Science, Japan

12:40 – 13:00 OP 14

Pressure dependency of azeotropic point for binary system methanol + dimethyl carbonate

Hiroyuki Matsuda*, Mitsuaki Negishi, Shinya Iino, Kiyofumi Kurihara, Katsumi Tochigi, Kenji Ochi

Nihon University, Japan

13:00 – 13:10 Closing Remarks and Student Poster Award

Prof. Kiyofumi Kurihara (Nihon University, Japan)

List of Poster Presentations

PP 01

CO₂ solubilities in ether functionalized phosphonium-based ionic liquids at 313.15 K

Kouta Takahashi¹, Takumi Takahashi¹, Masaki Watanabe¹, Daisuke Kodama^{*1}, Takashi Makino², Mitsuhiro Kanakubo², Tsutomu Watanabe³, Eri Hamanishi³

¹ Nihon University, Japan

² National Institute of Advanced Industrial Science and Technology (AIST), Japan

³ Nippon Chemical Industrial Co., Ltd., Japan

PP 02

Thermodynamic modeling of high pressure VLE and LLE for dimethylether + water system using equation of state

Shigeo Oba^{*1}, Tomoya Tsuji², Lian See Tan²

¹ Applied Thermodynamics and Physical Properties, Co., Ltd., Japan

² Universiti Teknologi Malaysia, Malaysia

PP 03

Characterization for structure-based CO₂ selectivity of ionic clathrate hydrates

Hidenori Hashimoto^{1,2}, Hiroyuki Ozeki¹, Sanehiro Muromachi^{*2}

¹ Toho University, Japan

² National Institute of Advanced Industrial Science and Technology (AIST), Japan

PP 04

Cross-correlation analysis of stress-structure coupling of liquids

Tsuyoshi Yamaguchi^{*}

Nagoya University, Japan

PP 05

CO₂ absorption effect on physical properties for butylethanolamine aqueous solution at 313 K

Kento Fujita¹, Masaki Okada¹, Taka-aki Hoshina^{*1}, Hidetaka Yamada², Tomoya Tsuji³, Toshihiko Hiaki¹

¹ Nihon University, Japan

² Reserch Institute of Innovative Technology for the Earth, Japan

³ Universiti Teknologi Malaysia, Malaysia

PP 06

Interfacial Tension of CO₂/EtOH/PS ternary system

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Measurement and correlation of vapor – liquid distribution coefficients of flavonoids in supercritical carbon dioxide – ethanol – water systems

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Memory effect and hydrate reformation from TBAB aqueous solution - SEM observation

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PVT relationships of methyltrimethoxysilane and tetramethyl orthosilicate

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A generalized model for predicting adsorption equilibria of various VOCs on activated carbon in supercritical carbon dioxide

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Phase equilibrium relations of semiclathrate hydrates based on tetra-*n*-butylphosphonium formate, acetate, propionate and lactate

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Representation of solubilities of phenylthioanthraquinone in supercritical carbon dioxide using Hansen solubility parameter

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Thermodynamic stabilities of tetra-*n*-butylphosphonium + gas semiclathrate hydrate systems

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Phase equilibrium measurement of semiclathrate hydrates by differential scanning calorimetry

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Densities for CO₂ / C₆H₁₂, C₆H₁₁CH₃ and C₂H₅C₆H₅ systems

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Development a new rolling ball viscometer for CO₂ expanded liquids

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Measurement and correlation of the SO₂/PEGDME system with activity coefficient models

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Continuous reactive crystallization of transparent oxide semiconductor CuAlO₂ in supercritical water

Takafumi Ueno, Toshiyuki Sato^{*}, Toshihiko Hiaki

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Effect of solid co-solvent addition on the glass transition temperature of pharmaceutical excipients under high pressure carbon dioxide

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Vapor pressure and liquid density of 1-butyl-3-methylimidazolium tetrafluoroborate + ammonia mixtures

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Prediction of solubility and diffusion coefficient of ethylene in propylene copolymers; extrapolation from molten state to rubbery state

Ayano Kitagishi, Suiri Takizawa, Yoshiyuki Sato^{*}, Hiroshi Inomata

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Measurement and modeling of infinite dilution activity coefficients for organic compounds in ionic liquid mixtures ([Bmim]Cl_{0.50}[Tf₂N]_{0.50})

Tomoka Shida, Yuya Hiraga, Takuya Sugiyama, Yoshiyuki Sato, Masaru Watanabe, Richard L. Smith, Jr.*

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Novel method for Screening hypertension suppressing substance from soybean milk protein

Ryunosuke Mitani*, Kenji Mishima, Tanjina Sharmin, Taku Michael Aida, Miyuki Nakamura

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Screening of phase separation solvent for CO₂ capture by COSMO-RS

Hiroshi Machida*, Mana Nakaoka, Tran Viet Bao Khuyen, Koyo Norinaga

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Development of measurement method for diffusion coefficients of nanoparticles by Taylor dispersion method

Naoya Tajima, Motoyuki Kimura, Daisuke Hojo, Gimyeong Seong, Tsutomu Aida, Akira Yoko, Takaaki Tomai, Tadafumi Adschiri*

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Dielectric properties of liquefied propane + alcohol mixtures at 303.2 K

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Measurement of solubility of TIPS-Pentacene in supercritical carbon dioxide by the determination of saturation states using UV-visible spectroscopy

Yusuke Shiba, Takanori Kobayashi, Hirohisa Uchida*

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Measurement of non-ideality of hansen solubility parameter for solvent mixture using physical properties

Takuya Tamura*, Hideki Yamamoto

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Measurement of isobaric vapor-liquid equilibrium and determination of azeotropic data for binary system 2-methyl-2-ethoxypropane (1) + ethanol (2) at 60.0 kPa and 101.3 kPa

Wakana Maeda¹, Toshiyuki Sato¹, Shigeo Oba², Toshihiko Hiaki^{*,1}

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Designing ionic liquids for efficient CO₂ capture: A materials informatics study

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Density, viscosity, and CO₂ solubility in deep eutectic solvents composed of quaternary ammonium salt and ethylene glycol

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CO₂ absorption and physical properties of tributylphosphonium benzotriazolates

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Oil phase swelling and extraction mechanism during supercritical fluid emulsion extraction via phase behavior observation

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Solvation structure and thermodynamics for rare earth complexes in ionic liquids evaluated by ADF and MD simulations

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Effect of gases and discharge product solubility inside cathode toward the advantages of ionic liquid in Li-O₂/CO₂ battery

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Effect of phosphonium ionic liquids on thermal stability of polymethyl methacrylate polymers

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Solvent polarity of alcohol and DBU mixtures switched by CO₂

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Antioxidant activity of nobiletin and tangeretin extracted from Genkou peels by optimized liquid carbon dioxide

Hiroyuki Tashiro, Ryunosuke Mitani, Shinichi Tokunaga, Masashi Haraguchi, Kenji Mishima^{*}, Tanjina Sharmin, Taku Michael Aida, Miyuki Nakamura

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Vapor-liquid equilibrium for binary systems containing 1,1,2,2-tetrafluoro-1-(2,2,2-trifluoroethoxy)ethane

Kaoru Yamaguchi^{*}, Shimpei Nagata, Hideo Ogawa, Fumio Kimura

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Amended experimental VLE and LLE data determined from the universal correlations of infinite dilution activity coefficients covering 5000 binaries

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Correlation and prediction of high-pressure binary VLE data above solute critical using the activity coefficients of hypothetical liquid

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Prediction of kinematic viscosities for ternary aqueous systems using modified Eyring and activity coefficient models

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Prediction of kinematic viscosities for ternary systems from binary data using Mcallister equation

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Carbon dioxide separation evaluated based on phase equilibria of CO₂ + N₂ + tetra-*n*-butylammonium bromide semi-clathrate hydrates

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Decomposition of methane hydrates analyzed with Raman spectroscopy and a mass transfer model considering cage occupancy

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Extraction of active ingredients from Magnoliae Cortex using supercritical carbon dioxide

Ding Dengpei, Jun Endo, Hiroyuki Matsuda^{*}, Kiyofumi Kurihara, Katsumi Tochigi
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The role of water on alanine condensation in high temperature water: a DFT and Monte Carlo study

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Measuring the effects of citrus fruits on cerebral blood flow by using fNIRS

Masashi Haraguchi^{*}, Kenji Mishima, Taku M. Aida, Tanjina Sharmin, Miyuki Nakamura, Hiroyuki Tashiro

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Supercritical fluid-assisted formation of Pd-Ru bimetallic nanoparticles

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Shinichi Tokunaga, Kenji Mishima*, Tanjina Sharmin, Taku Michael Aida, Miyuki Nakamura
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Reaction kinetics of ester hydrolysis and solvolysis in hot compressed water-methanol mixed solvents

Makoto Akizuki*, Kohki Ito, Yoshito Oshima
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Utilization of micro-mixing technique containing supercritical CO₂-water fluids for extraction of ferulic acid from the aqueous solution

Peany Houng, Yuya Murakami, Yusuke Shimoyama*
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Investigation and improvement of the structure stability of H-ZSM-5 in sub- and supercritical water

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Reorientational dynamics and liquid structure in liquefied propane – alcohol mixtures

Masaki Okada*¹, Yusuke Koshiba¹, Taka-aki Hoshina¹, Tomoya Tsuji², Toshihiko Hiaki¹
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Encapsulation of silica hollow microspheres with pH responsive polymer by pressure-induced phase separation of CO₂ Solution

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Mechanism of optical rotation reduction for sugar solution during microwave irradiation

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Special behavior for surface tension of alcohol aqueous solution by microwave irradiation

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Flow synthesis of silver nanoparticles and its characterization of optical property

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Modified Hansen Solubility Sphere Method based on Solid Reference Materials

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Accurate calculation of physical properties of materials with QM and MD simulations

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Development of automatic phase separation recognition method by image processing

Eito Arita, Daiki Nakamura, Makoto Misumi, Hideaki Orii, Kenji Mishima^{*}, Tanjina Sharmin, Taku Micheal Aida, Miyuki Nakamura

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Morphological changes in polyethylene upon melting investigated by *in situ* Raman spectroscopy

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Insights into the mechanism of the acid-catalyzed hydrolysis of hesperidin using quantum chemical calculations

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The infinite dilution partial molar volumes of lipids in supercritical CO₂

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Synthesis of graphene using plasma-assisted CVD method at low temperature

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