



MTMS '21

9th International Symposium on
Molecular **T**hermodynamics and
Molecular **S**imulation

Program Book



September 7-9, 2021

Virtual



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Molecular Simulation**

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写真：暁の伊達政宗公 写真提供：宮城県観光プロモーション推進室



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.) Prof. Richard L. Smith (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.)
8 th	2018	Narashino	-Prof. Kiyofumi Kurihara (Nihon Univ.)

The 9th International Symposium on “Molecular Thermodynamics and Molecular Simulation (MTMS’21)” is held during September 7-9, 2021 on virtual. 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, 7 keynote lectures by eminent scientists and engineers, 11 invited lectures on selected topics, 17 oral presentations, and 32 poster presentations with flash talk.

At this MTMS, as with the 3rd MTMS, we planned to gather at a hotel in Akiu hot springs, Sendai, to deepen discussions and friendships. The current situation in Japan is that the spread of COVID-19 has not stopped and a state of emergency has been issued in some areas. Although it was a very short preparation period, we can hold MTMS as an online conference with the cooperation of many people concerned.

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

We hope all the participants will enjoy the symposium.

Yoshiyuki Sato
Mitsuhiro Kanakubo
Symposium Chair



Organizing Committees

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Bastian Schmid (DDBST, Germany)
Gang Xu (AVEVA, U.K.)



Timetable

September 7, 2021 (Tuesday)

8:40 – 8:50	Opening Remarks
8:50 – 10:40	Session I IL 01, OP 01, OP 02, OP 03, OP 04
10:40 – 11:00	Coffee Break
11:00 – 11:50	Session II IL 02, OP 05
11:50 – 13:20	Lunch
13:20 – 15:10	Session III IL 03, OP 06, OP 07, OP 08, OP 09
15:10 – 15:30	Coffee Break
15:30 – 16:30	Session IV OP 10, OP 11, OP 12
16:30 – 16:50	Coffee Break
16:50 – 18:50	Session V KL 01, KL 02, KL 03

September 8, 2021 (Wednesday)

8:20 – 9:30	Session VI KL 04, IL 04
9:30 – 9:50	Coffee Break
9:50 – 11:20	Session VII IL 05, OP 13, KL 05
11:20 – 13:00	Lunch
13:00 – 15:10	Session VIII IL 06, IL 07, IL 08, KL 06
15:10 – 15:40	Coffee Break
15:40 – 17:30	Session IX IL 09, OP 14, OP 15, OP 16, OP 17
17:30 – 17:50	Coffee Break
17:50 – 19:20	Session X IL 10, PL 01

Poster sessions are available from 10:00 on September 6 to 17:00 on September 9 (JST).

Participants can view posters and ask questions via chat.

September 9, 2021 (Thursday)

8:20 – 9:30	Session XI		IL 11, KL 07	
9:30 – 9:40	Coffee Break			
9:40 – 12:20	Poster Session with Flash Talk			
	Room A		Room B	
9:40 – 10:40	PA 01 – PA 06	9:40 – 10:40	PB 01 – PB 06	
10:40 – 11:05	PA 01 – PA 06 Questions	10:40 – 11:05	PB 01 – PB 06 Questions	
11:05 – 11:10	Break	11:05 – 11:10	Break	
11:10 – 12:00	PA 07 – PA 11	11:10 – 12:00	PB 07 – PB 11	
12:00 – 12:20	PA 07 – PA 11 Questions	12:00 – 12:20	PB 07 – PB 11 Questions	
12:20 – 13:30	Lunch			
13:30 – 14:40	Poster Session with Flash Talk			
	Room A		Room B	
13:30 – 14:20	PA 12 – PA 16	13:30 – 14:20	PB 12 – PB 16	
14:20 – 14:40	PA 12 – PA 16 Questions	14:20 – 14:40	PB 12 – PB 16 Questions	
14:40 – 14:50	Break			
14:50 – 15:10	Closing Remarks			
	Student Presentation Award			

Poster sessions are available from 10:00 on September 6 to 17:00 on September 9 (JST).

Participants can view posters and ask questions via chat.

September 7, Tuesday				September 8, Wednesday				September 9, Thursday			
Time	Number	Presenter	Chair	Time	Number	Presenter	Chair	Time	Number	Presenter	Chair
8:40		Opening Remarks		8:20	KL04	C. M ^c Cabe	H. Matsuda	8:20	IL11	C.-C. Chen	S. Oba
8:50	IL01	T. Hiaki		9:00	IL04	G. Xu	H. Mori	8:50	KL07	Y. Iwai	T. Furuya
9:20	OP01	H. Matsuda		9:30		Coffee Break		9:30		Coffee Break	
9:40	OP02	T. Funazukuri	K. Mishima	9:50	IL05	S.-T. Lin	G. Xu	9:40		Poster Session with Flash Talk	
10:00	OP03	S. Ohe	I. Ushiki	10:20	OP13	H. Mori	T. Tsuji			Room A: PA01 - PA11	
10:20	OP04	M. Osada		10:40	KL05	P. Cummings		12:20		Room B: PB01 - PB11	
10:40		Coffee Break		11:20		Lunch		12:20		Lunch	
11:00	IL02	H. Inomata	Y. Sato	13:00	IL06	T. Tsuji		13:30		Poster Session with Flash Talk	
11:30	OP05	I. Ushiki	M. Osada	13:30	IL07	E. May	S.-T. Lin			Room A: PA12 - PA16	
11:50		Lunch		14:00	IL08	K. Shin	H. Yamada	14:40		Room B: PB12 - PB16	
13:20	IL03	R. Smith		14:30	KL06	V. K. Rattan		14:40		Break	
13:50	OP06	Y. C. Hung		15:10		Coffee Break		14:50		Closing Remarks	
14:10	OP07	A. Duereh	T. Hoshina	15:40	IL09	H. Yamada				Student Presentation Award	
14:30	OP08	A. R. Agustin	H. Machida	16:10	OP14	H. Machida	D. Kodama	PL**		Plenary Lecture	
14:50	OP09	Y. Orita		16:30	OP15	T. Yamaguchi	T. Furuya	KL**		Keynote Lecture	
15:10		Coffee Break		16:50	OP16	K. Tran		IL**		Invited Lecture	
15:30	OP10	S. Tokunaga		17:10	OP17	H. Nishiumi		OP**		Oral Presentation	
15:50	OP11	K. Mishima	A. Soto	17:30		Coffee Break		PA**		Poster Presentation	
16:10	OP12	T. Sato	A. Duereh	17:50	IL10	B. Schmid	H. Inomata	PB**		Poster Presentation with Flash Talk	
16:30		Coffee Break		18:20	PL01	G. M. Kontogeorgis	M. Sasaki			Last Update	2021/8/26
16:50	KL01	I. G. Economou	Y. Iwai								
17:30	KL02	A. Soto	R. Smith								

PA or PB**** Chat discussions are available from 10:00 on September 6 to 17:00 on September 9 (JST).

September 9, Thursday

Room A						Room B			
Time	Number	Presenter	Chair	Time	Number	Presenter	Chair		
9:40	PA01	T. Yamada	T. Makino M. Ota	9:40	PB01	Y. Aina	T. Sato T. Honma		
9:50	PA02	T. Tachibana		9:50	PB02	Y. Suzuki			
10:00	PA03	J. Shimada		10:00	PB03	R. Kinoshita			
10:10	PA04	K. Ikeda		10:10	PB04	T. Igosawa			
10:20	PA05	S. Akiyama		10:20	PB05	A. Legaspi			
10:30	PA06	Y. Tatsumi		10:30	PB06	N. Maeda			
10:40	PA	Questions 25 min.	10:40	PB	Questions 25 min.				
11:05		Break	11:05		Break				
11:10	PA07	A. Tokoro	M. Kanakubo S. Muromachi	11:10	PB07	K. Matsubara	T. Sugahara C. Y. Kong		
11:20	PA08	M. Yomori		11:20	PB08	R. Suzuki			
11:30	PA09	T. Homma		11:30	PB09	M. Kitahara			
11:40	PA10	T. Wijakmatee		11:40	PB10	T. Kataoka			
11:50	PA11	T. Maeda		11:50	PB11	Y. Hao			
12:00	PA	Questions 20 min.		12:00	PB	Questions 20 min.			
12:20		Lunch	12:20		Lunch				
13:30	PA12	M. Ota	Y. Shimoyama H. Miyamoto	13:30	PB12	T. Makino	H. Uchida M. Akizuki		
13:40	PA13	K. Tochigi		13:40	PB13	T. Sugahara			
13:50	PA14	Y. Asakuma		13:50	PB14	C. Y. Kong			
14:00	PA15	T. Hoshina		14:00	PB15	T. Honma			
14:10	PA16	K. Tochigi		14:10	PB16	J. L. Lee			
14:20	PA	Questions 20 min.		14:20	PB	Questions 20 min.			
Last Update			2021/8/19						



General Information

Web Conference System

MTMS '21 will be held using Zoom and web conference system shown in the image below. Participants can access Zoom link, abstract, proceedings, e-poster, chat, etc. using this web conference system. Further information will be uploaded in the MTMS '21 website <https://mtms21.jimdofree.com/>.

9th International Symposium on Molecular Thermodynamics and Molecular Simulation (MTMS'21)

Demo Program [Program Book](#)

Poster Session with Flash Talk [Logout](#)

Please note that for all participants, this conference will be held in **Room A** for the purpose of archiving the event for official purposes. Participants must not record lectures at the conference. Poster sessions are available from 10:00 on September 6 to 17:00 on September 9 (JST). Participants can view posters and ask questions via chat.

Oral [Poster A](#) [Poster B](#)

Time	September 7, Tuesday	Chair	Time	September 8, Wednesday	Chair	Time	September 9, Thursday	Chair
08:40-08:50	Opening Remarks		08:20-09:00	KL04 C. McCabe	H. Matsuda H. Mori	08:20-08:50	IL11 C.-C. Chen	S. Oba T. Furuya
08:50-09:20	IL01 T. Hiaki		09:00-09:30	IL04 G. Xu		08:50-09:30	KL07 Y. Iwai	
09:20-09:40	OP01 H. Matsuda		09:30-09:50	Coffee Break		09:30-09:40	Coffee Break	
09:40-10:00	OP02 T. Funazukuri	K. Mishima I. Ushiki	09:50-10:20	IL05 S.-T. Lin		09:40-11:05	Poster Session Room A: PA01 - PA11 Room B: PB01 - PB11	

9th International Symposium on Molecular Thermodynamics and Molecular Simulation (MTMS'21)

Demo **Plenary, Keynote, Invited Lectures** [Close](#)
Oral Presentations

Recording, taking screen shots, photos, or archiving materials is strictly prohibited.

Zoom Link

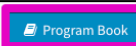

Abstract **Proceeding**
Chat

September 7, Tuesday

08:40~08:50	Session 1 : Opening Remarks Prof. Yoshiyuki Sato (Tohoku Institute of Technology, Japan) Dr. Mitsuhiro Kanakubo (National Institute of Advanced Industrial Science and Technology, Japan)	
08:50~10:40	Session 2 : Session I Chair: Prof. Kenji Mishima (Fukuoka University, Japan) and Prof. Ikuo Ushiki (Hiroshima University, Japan)	
08:50~09:20	Measurement of vapor-liquid equilibria for azeotropic systems Toshihiko Hiaki* Nihon University, Japan	
09:20~09:40	Phase diagram of ternary mixtures water + n-alkane + non-ionic surfactant Hiroyuki Matsuda ^{1,2} , Yuki Nakazato ¹ , Rei Tsuchiya ¹ , Yoshihiro Inoue ¹ , Kiyofumi Kurihara ¹ , Tomoya Tsuji ² , Katsumi Tochigi ¹ , Kenji Ochi ¹ ¹ Nihon University, Japan ² Universiti Teknologi Malaysia, Malaysia	

9th International Symposium on Molecular Thermodynamics and Molecular Simulation (MTMS'21)

Demo ~~Poster Presentation with Flash Talk~~

Program Book  

Recording, taking screen shots, photos, or archiving materials is strictly prohibited.


Oral Poster A **Poster B**

number	Title	
num. search	Title search	Proceeding
Poster Session with Flash Talk Chair: Prof. Masaki Ota (Tohoku University, Japan) and Dr. Takashi Makino (National Institute of Advanced Industrial Science and Technology, Japan)		
PA01 09:40-09:50	Measurements and Modeling of Vapor-Liquid Equilibrium Properties for Low GWP refrigerants R1123/R1234yf/R32 Ternary Mixtures Tessei Yamada, Yuuhei Nakamura, Kyouhei Minai, Hiroyuki Miyamoto* Toyama Prefectural University, Japan	e-Poster Movie Chat Proceeding
PA02 09:50-10:00	Phase Behavior of CO₂/Toluene/PMMA ternary system Takumi Tachibana, Hiroaki Matsukawa, Yuya Murakami, Atsushi Shono, Katsuto Otake* Tokyo University of Science, Japan	Poster Movie Chat Proceeding
PA03 10:00-10:10	Thermodynamic properties of tetra-n-butylphosphonium dicarboxylate semicrathrate hydrates Jin Shimada ¹ , Moe Yamada ² , Takeshi Sugahara ^{1,3} , Atsushi Tani ³ , Katsuhiko Tsunashima ² , Takayuki Hirai ¹ ¹ Osaka University, Japan ² National Institute of Technology, Wakayama Collage, Japan ³ Kobe University, Japan	Poster Movie Chat Proceeding

OP01
Phase diagram of ternary mixtures water + n-alkane + non-ionic surfactant


Hiroyuki Matsuda^{*,1}, Yuki Nakazato¹, Rei Tsuchiya¹, Yoshihiro Inoue¹, Kiyofumi Kurihara¹, Tomoya Tsuji², Katsumi Tochigi¹, Kenji Ochi¹
¹Nihon University, Japan ²Universiti Teknologi Malaysia, Malaysia

Enter question

Question from Participants 

Demo **Chat Discussion**

Enter reply

Answer from authors 

Attention

1. Presentation materials should be treated as public announcements that may affect future intellectual property rights such as patents. If you agree that the video files are to be downloaded by participants, then please upload your presentation materials at your discretion.
2. Downloaded files must only be used for personal reasons and must not be shared or stored on file servers. All files must be deleted from all digital devices including disk caches immediately after the end of the MTMS symposium.
3. Please note that for all participants and events, this conference will be recorded for the purpose of archiving the event for official purposes. Participants must not record lectures at the conference.

Instructions for Presenter

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

Authors should prepare oral presentations with a total duration of 60 minutes (plenary lecture), 40 minutes (keynote lecture), 30 minutes (invited lecture), or 20 minutes (oral presentation) including questions (approx. 4 or 5 minutes per talk).

2. Poster Presentation with Flash Talk

- (1) Chat discussions throughout a certain period in the symposium are available.
- (2) Flash talk is held on September 9. Please check Program.
- (3) Authors should prepare an oral presentation with 10 minutes.
- (4) Time of questions for 5 to 6 talks will be 20 to 25 minutes.
- (5) Poster and movie file
 - The poster presenter has to submit the poster file.
 - Submission of poster presentation movie file is optional.
 - The poster file is required to be submitted as PDF (Portable Document Format) file.
 - The movie file is required to be submitted as MP4 file.
 - The organizing committee recommend, for the ease of viewing on screen, that the poster PDF file is containing about 10 sheets of slideshow.
 - Please submit your poster and movie files via Online Submission Form by September 1, 2021.
 - Further information will be uploaded in the MTMS '21 website <https://mtms21.jimdofree.com/>.

Student Presentation Award

Undergraduate/graduate student presenters are considered for the student presentation award. Award ceremony will be held in the closing remarks on September 9.

Special Issue

We are pleased to announce a special issue of the 9th International Symposium on Molecular Thermodynamics and Molecular Simulation (MTMS '21) in the journal *Fluid Phase Equilibria* that will be edited by Prof. Yoshiyuki Sato and Dr. Mitsuhiro Kanakubo as guest-editors.

We invite all conference participants to submit a manuscript for publication in the special issue. Please note that all submissions must comply with the scope of *Fluid Phase Equilibria* and will be peer reviewed in the same manner as all other articles published in *Fluid Phase Equilibria*.

We are excited about this special issue and will do our utmost to ensure timely reviewing and publication.



Technical Program

11:30 – 11:50	OP 05
Predicting the solubilities of acetylacetonate-type metal precursors in supercritical CO₂: Thermodynamic modeling using PC-SAFT	
<u>Ikuo Ushiki</u> [*] , Ryo Fujimitsu, Azusa Miyajima, Shigeki Takishima Hiroshima University, Japan	
11:50 – 13:20	Lunch
13:20 – 15:10	Session III
Chair: Prof. Taka-aki Hoshina (Nihon University, Japan) and Prof. Hiroshi Machida (Nagoya University, Japan)	
13:20 – 13:50	Invited Lecture IL 03
Application of analytical centrifugation to chemical systems for measurement of properties and phase equilibria	
Kotaro Oshima, Kentaro Nakamura, Natsuki Sato, Haixin Guo and <u>Richard Lee Smith Jr.</u> [*] Tohoku University, Japan	
13:50 – 14:10	OP 06
Controlling the CO₂-lipid liquid phase separation via process tuning and lipid structural design	
<u>Ying-Chieh Hung</u> ¹ , Yuna Tatsumi ¹ , Chieh-Ming Hsieh ² , Shiang-Tai Lin ³ , Yusuke Shimoyama ^{*,1} ¹ Tokyo Institute of Technology, Japan ² National Central University, Taiwan ³ National Taiwan University, Taiwan	
14:10 – 14:30	OP 07
Development of CO₂-assisted dispersibility of organic-inorganic hybrid nanoparticles with expanded liquid solvent mixtures	
<u>Alif Duereh</u> ^{*,1} , Masaki Ota ¹ Yoshiyuki Sato ² , Hiroshi Inomata ¹ ¹ Tohoku University, Japan ² Tohoku Institute of Technology, Japan	
14:30 – 14:50	OP 08
Surface modification of nano-TiO₂ with para-aminobenzoic acid in supercritical carbon dioxide for preventing aggregation of nanoparticles	
<u>Anggi Regiana Agustin</u> , Kazuhiro Tamura [*] Kanazawa University, Japan	
14:50 – 15:10	OP 09
Synthesis of decanoic acid-modified iron oxide nanocrystals using supercritical carbon dioxide as reaction medium	
<u>Yasuhiko Orita</u> [*] , Keito Kariya, Thossaporn Wijakmatee, Yusuke Shimoyama Tokyo Institute of Technology, Japan	
15:10 – 15:30	Coffee Break
15:30 – 16:30	Session IV
Chair: Prof. Ana Soto (Universidade de Santiago de Compostela, Spain) and Prof. Alif Duereh (Tohoku University, Japan)	

15:30 – 15:50	OP 10
Production of spherical microparticles with Eudragit L100 by the PGSS process in supercritical CO₂-ethanol mixtures	
<u>Shinichi Tokunaga</u> , Miyuki Nakamura, Tanjina Sharmin, Taku M. Aida, Kenji Mishima*	
Fukuoka University, Japan	
15:50 – 16:10	OP 11
Application of direct sonication under high-pressure two-phase system	
<u>Kenji Mishima</u> *, Tanjina Sharmin, Taku Michael Aida, Kento Ono	
Fukuoka University, Japan	
16:10 – 16:30	OP 12
Analysis of the mechanism of hydrothermal carbon dioxide fixation into serpentine with estimation of equilibrium of chemical species	
<u>Takafumi Sato</u> *, Seitaro Yamamoto, Naotsugu Itoh	
Utsunomiya University, Japan	
16:30 – 16:50	Coffee Break
16:50 – 18:10	Session V
Chair: Prof. Yoshio Iwai (Kyushu University, Japan) and Prof. Richard L. Smith (Tohoku University, Japan)	
16:50 – 17:30	Keynote Lecture KL 01
Clean, high quality low emission fuels with Fischer-Tropsch synthesis: A multiscale study of transport properties in confined systems	
<u>Ioannis G. Economou</u> ^{*1,2} , Konstantinos D. Papavasileiou ¹ , Loukas D. Peristeras ¹ Andreas Bick ³	
¹ Institute of Nanoscience and Nanotechnology, Greece	
² Texas A&M University at Qatar, Qatar ³ Scienomics SAS, France	
17:30 – 18:10	Keynote Lecture KL 02
Phase equilibria and enhanced oil recovery	
Ana Soto*	
Universidade de Santiago de Compostela, Spain	
18:10 – 18:50	Keynote Lecture KL 03
	Cancelled
Applications of deep eutectic solvents and gas hydrates in gas purifications	
Samah E. E. Warrag ^{1,2} , Muhammad Naveed Khanc ^{3,4} , <u>Cor J. Peters</u> ^{*,1,2,4}	
¹ Khalifa University of Science and Technology, United Arab Emirates	
² Eindhoven University of Technology, The Netherlands	
³ University of Hafr Al Batin, Kingdom of Saudi Arabia ⁴ Colorado School of Mines, USA	

Tomoya Tsuji*¹, Junya Yamada², Midori Kawasaki², Machie Otsuka², Atsushi Kobayashi²

¹ Universiti Teknologi Malaysia, Malaysia ² INPEX Corporation, Japan

13:30 – 14:00 Invited Lecture IL 07

Solids formation risk in natural gas, LNG and liquid hydrogen production

Eric F. May*^{1,2}, Peter Metaxas¹, Paul Stanwix¹, Peter Falloon¹, Vincent Lim¹, Matthew Hopkins¹, Catherine Sampson¹, Arman Siahvashi¹, Zachary Aman¹

¹ The University of Western Australia, Australia

² Future Energy Exports Cooperative Research Centre, Australia

14:00 – 14:30 Invited Lecture IL 08

Molecular behavior of 1-pentanol guest in the NH₄F-doped clathrate hydrate

Byeongwan Lee^{1,2}, Jeongtak Kim^{1,3}, Kyuchul Shin*¹, Ki Hun Park⁴, Minjun Cha⁴, Saman Alavi*^{5,6}, John A. Ripmeester⁶

¹ Kyungpook National University, Republic of Korea

² Korea Atomic Energy Research Institute, Republic of Korea

³ Korea Institute of Energy Research, Republic of Korea

⁴ Kangwon National University, Republic of Korea

⁵ University of Ottawa, Canada ⁶ National Research Council of Canada, Canada

14:30 – 15:10 Keynote Lecture KL 06

Kinetic viscosities prediction using ASOG-VISCO group contribution method for binary liquid mixtures

V. K. Rattan*¹, Hiroyuki Matsuda², Katsumi Tochigi², Kiyofumi Kurihara², Toshitaka Funazukuri³

¹ GNA University, India

² Nihon University, Japan

³ Chuo University, Japan

15:10 – 15:40 Coffee Break

15:40 – 17:30 Session IX

Chair: Prof. Daisuke Kodama (Nihon University, Japan) and Dr. Takeshi Furuya (National Institute of Advanced Industrial Science and Technology, Japan)

15:40 – 16:10 Invited Lecture IL 09

Physical chemistry of amine-based carbon dioxide separation

Hidetaka Yamada*

Kanazawa University, Japan

16:10 – 16:30 OP 14

High throughput CO₂ solubility measurement in amine solution using HS-GC

Hiroshi Machida*, Keiichi Yanase, Tran Viet Bao Khuyen, Mikiro Hirayama, Koyo Norinaga

Nagoya University, Japan

16:30 – 16:50 OP 15

A new approach to the study of amine-CO₂ system based on the absolute reaction rate theory

Toru Yamaguchi*¹, Hidetaka Yamada², Syohei Sanada¹, Kenji Hori^{1,3}

¹ Transition State Technology Co. Ltd., Japan

² Kanazawa University, Japan

³ Yamaguchi University, Japan

16:50 – 17:10 **OP 16**

Temperature dependent of absorption heat in phase-change solvent in carbon dioxide capture

Tran Viet Bao Khuyen, Yamaguchi Tsuyoshi, Machida Hiroshi*, Koyo Norinaga

Nagoya University, Japan

17:10 – 17:30 **OP 17**

Prediction of CO₂ solubility in ionic liquids and glymes with modified generalized BWR Eos

Hideo Nishiumi*¹, Daisuke Kodama²

¹ Hosei University, Japan

² Nihon University, Japan

17:30 – 17:50 Coffee Break

17:50 – 19:20 **Session X**

Chair: Prof. Hiroshi Inomata (Tohoku University, Japan) and Dr. Masakazu Sasaki (Toyo Engineering Co, Japan)

17:50 – 18:20 **Invited Lecture IL 10**

DDBST and LTP – Your source for reliable thermophysical properties

Bastian Schmid*

DDBST GmbH, Germany

18:20 – 19:20 **Plenary Lecture PL 01**

How can molecular concepts help in the development of more predictive advanced equations of state?

Georgios M. Kontogeorgis*, Xiaodong Liang

Technical University of Denmark, Denmark

September 9, 2021 (Thursday)

8:20 – 9:30	Session XI
Chair: Dr. Shigeo Oba (Applied Thermodynamics and Physical Properties Co., Ltd., Japan) and Dr. Takeshi Furuya (National Institute of Advanced Industrial Science and Technology, Japan)	
8:20 – 8:50	Invited Lecture IL 11
Association-based activity coefficient models for nonelectrolyte and electrolyte solutions	
Chau-Chyun Chen* Texas Tech University, USA	
8:50 – 9:30	Keynote Lecture KL 07
Prediction of vapor-liquid equilibria for multicomponent systems by a modified concentration dependent surface area parameter model	
Yoshio Iwai* Kyushu University, Japan	
9:30 – 9:40	Coffee Break
9:40 – 11:05	Poster Session with Flash Talk Room A
Chair: Prof. Masaki Ota (Tohoku University, Japan) and Dr. Takashi Makino (National Institute of Advanced Industrial Science and Technology, Japan)	
9:40 – 9:50	PA 01
Measurements and modeling of vapor-liquid equilibrium properties for low GWP refrigerants R1123/R1234yf/R32 ternary mixtures	
<u>Tessei Yamada</u> , Yuuhei Nakamura, Kyouhei Minai, Hiroyuki Miyamoto* Toyama Prefectural University, Japan	
9:50 – 10:00	PA 02
Phase behavior of CO₂/toluene/PMMA ternary system	
<u>Takumi Tachibana</u> , Hiroaki Matsukawa, Yuya Murakami, Atsushi Shono, Katsuto Otake* Tokyo University of Science, Japan	
10:00 – 10:10	PA 03
Thermodynamic properties of tetra-<i>n</i>-butylphosphonium dicarboxylate semiclathrate hydrates	
<u>Jin Shimada</u> ¹ , Moe Yamada ² , Takeshi Sugahara ^{*1} , Atsushi Tani ³ , Katsuhiko Tsunashima ² , Takayuki Hirai ¹ ¹ Osaka University, Japan ² National Institute of Technology, Wakayama Collage, Japan ³ Kobe University, Japan	
10:10 – 10:20	PA 04
Gas separation properties of semiclathrate hydrates for CH₄+CO₂ mixed gas	
<u>Kosuke Ikeda</u> ¹ , Takuya Yasoyama ¹ , Hiroyuki Miyamoto ^{*1} , Sanehiro Muromachi ² ¹ Toyama Prefectural University, Japan ² National Institute of Advanced Industrial Science and Technology, Japan	
10:20 – 10:30	PA 05

Host-guest chemistry of antibacterial molecular crystal in supercritical CO₂ with solvent

Seika Akiyama^{*}, Yingquan Hao, Yusuke Shimoyama

Tokyo Institute of Technology, Japan

10:30 – 10:40 PA 06

Itraconazole cocrystallization in fatty acid under high-pressure CO₂

Yuna Tatsumi, Hao Yingquen, Yasuhiko Orita, Yusuke Shimoyama^{*}

Tokyo Institute of Technology, Japan

10:40 – 11:05 PA 01 – PA 06 Questions

9:40 – 11:05 Poster Session with Flash Talk Room B

Chair: Prof. Takafumi Sato (Utsunomiya University, Japan) and Prof. Tetsuo Honma (National Institute of Technology (KOSEN), Hachinohe College, Japan)

9:40 – 9:50 PB 01

CO₂ solubility of deep eutectic solvent consisting of choline chloride and ethylene glycol

Yuto Ainai, Ayaka Taniguchi, Daisuke Kodama^{*}

Nihon University, Japan

9:50 – 10:00 PB 02

CO₂/hydrocarbon selectivity of phosphonium based ionic liquids

Yuki Suzuki¹, Daisuke Kodama^{*1}, Hirotohi Mori^{2,3}, Nahoko Kuroki^{2,4}, Hidetaka Yamada⁵

¹Nihon University, Japan ² Chuo University, Japan

³ Institute for Molecular Science, Japan

⁴ JST, ACT-X, Japan ⁵ Kanazawa University, Japan

10:00 – 10:10 PB 03

Thermodynamic study of extraction behavior for precious metals using phosphonium-based ionic liquids

Ryoma Kinoshita¹, Yusuke Tsuchida¹, Masahiko Matsumiya^{*1}, Yuji Sasaki²

¹ Yokohama National University, Japan ² Japan Atomic Energy Agency, Japan

10:10 – 10:20 PB 04

Thermodynamic study of W(VI) extraction using amine-based extractant and phosphonium ionic liquids

Tatsuki Igosawa¹, Yusuke Tsuchida¹, Masahiko Matsumiya^{*1}, and Yuji Sasaki²

¹ Yokohama National University, Japan ² Japan Atomic Energy Agency, Japan

10:20 – 10:30 PB 05

Effects of water in the decarboxylation of aromatic carboxylic acids in supercritical water

Anna Legaspi^{*}, Makoto Akizuki, Yoshito Oshima

The University of Tokyo, Japan

10:30 – 10:40 PB 06

Calculation of solubility of organic compounds in supercritical carbon dioxide using machine learning with molecular descriptors

Naoya Maeda, Junichi Sakabe, Hirohisa Uchida^{*}

Kanazawa University, Japan

10:40 – 11:05 PB 01 – PB 06 Questions

11:05 – 11:10	Break
11:10 – 12:20	Poster Session with Flash Talk Room A
Chair: Dr. Mitsuhiro Kanakubo (National Institute of Advanced Industrial Science and Technology, Japan) and Dr. Sanehiro Muromachi (National Institute of Advanced Industrial Science and Technology, Japan)	
11:10 – 11:20	PA 07
Volumetric behavior of HFO-1234ze(E) + acetone liquid mixture at 303.2 K	
<u>Atuski Tokoro</u> ¹ , Masaki Okada ¹ , Taka-aki Hoshina ^{*,1} , Tomoya Tsuji ² , Takeshi Furuya ³	
¹ Nihon University, Japan	
² Universiti Teknologi Malaysia (UTM) Kuala Lumpur, Malaysia	
³ The National Institute of Advanced Industrial Science and Technology (AIST), Japan	
11:20 – 11:30	PA 08
Measurement of the density of carbon dioxide/methanol and dioxide/ethanol homogeneous mixtures and correlation with equations of state	
<u>Masamune Yomori</u> ¹ , Hiroaki Matsukawa ¹ , Yuya Murakami ² , Atsushi Shono ¹ , Tomoya Tsuji ² , Katsuto Otake ^{*,1}	
¹ Tokyo University of Science, Japan ² University Technology Malaysia, Malaysia	
11:30 – 11:40	PA 09
Measurement and correlation of PVT for organic-inorganic hybrid nanoparticles	
<u>Taiki Homma</u> ^{*,1} , Masaki Ota ¹ , Yoshiyuki Sato ^{1,2} , Hiroshi Inomata ¹	
¹ Tohoku University, Japan ² Tohoku Institute of Technology, Japan	
11:40 – 11:50	PA 10
Micro-flow process of emulsification and supercritical fluid extraction of emulsion for stearic acid lipid nanoparticle production	
<u>Thossaporn Wijakmatee</u> , Yasuhiko Orita, Yusuke Shimoyama [*]	
Tokyo Institute of Technology, Japan	
11:50 – 12:00	PA 11
Study for hydration structure through the refractive index during microwave irradiation	
<u>Tomoisa Maeda</u> ¹ , Yusuke Asakuma ^{*,1} , Shinya Ito, Shuji Taue ² , Anita Hyde ³ , Chi Phan ³	
¹ University of Hyogo, Japan ² Kouchi Institute of Technology	
³ Curtin University, Australia	
12:00 – 12:20	PA 07 – PA 11 Questions
11:10 – 12:20	Poster Session with Flash Talk Room B
Chair: Prof. Takeshi Sugahara (Osaka University, Japan) and Prof. Chang Yi Kong (Shizuoka University, Japan)	
11:10 – 11:20	PB 07
Simultaneous correlation of liquid-liquid equilibria for ternary systems and phase equilibria for constitutive binary systems by modified new activity coefficient model	
<u>Koji Matsubara</u> , Yoshio Iwai [*]	
Kyushu University, Japan	
11:20 – 11:30	PB 08

Anionic states play more important role: electronic structure informatics of gas-phase acidity toward fast and precise acids design for engineering

Rima Suzuki¹, Nahoko Kuroki^{1,2}, Hirotohi Mori^{*1,3}

¹ Chuo University, Japan ² JST, ACT-X, Japan

³ Institute for Molecular Science, Japan

11:30 – 11:40 PB 09

Optimization of an artificial neural network for pure component parameters based on a group contribution method of PC-SAFT EoS

Masayuki Kitahara, Hiroaki Matsukawa, Yuya Murakami, Atsushi Shono, Katsuto Otake^{*2}

Tokyo University of Science, Japan

11:40 – 11:50 PB 10

Screening of phase-separation CO₂ absorbent using machine learning combined with molecular information

Taishi Kataoka, Yingquan Hao, Ying-Chieh Hung, Yusuke Shimoyama^{*}

Tokyo Institute of Technology, Japan

11:50 – 12:00 PB 11

Prediction of melting point and fusion enthalpy of cocrystal by machine learning combined with molecular informatics

Yingquan HAO, Yusuke Shimoyama^{*}

Tokyo Institute of Technology, Japan

12:00 – 12:20 PB 07 – PB 11 Questions

12:20 – 13:30 Lunch

13:30 – 14:40 Poster Session with Flash Talk Room A

Chair: Prof. Yusuke Shimoyama (Tokyo Institute of Technology, Japan) and Prof. Hiroyuki Miyamoto (Toyama Prefectural University, Japan)

13:30 – 13:40 PA 12

Development of a predictive dimensionless distribution coefficient (pDD) model for fractionation of Hops extracts

Masaki Ota^{*1}, Aruto Kuwahara¹, Yuki Hoshino¹, Yusuke Ueno¹, Shun Nomura¹, Yoshiyuki Sato^{1,2}, Richard Lee Smith Jr.¹, Hiroshi Inomata¹

¹ Tohoku University, Japan

² Tohoku Institute of Technology, Japan

13:40 – 13:50 PA 13

Evaluation of solid-liquid equilibria for drug + water + cyclodextrin derivatives systems using activity coefficient model

Hiroyuki Matsuda, Kiyofumi Kurihara, Katsumi Tochigi^{*}

Nihon University, Japan

13:50 – 14:00 PA 14

Prediction for modification of liquid-liquid interface by energy concentration of microwave heating

Yusuke Watanabe¹, Yosuke Shibata¹, Satoshi Sonobe¹, Yusuke Asakuma^{*1}, Anita Hyde², Chi Phan²

¹ University of Hyogo, Japan

² Curtin University, Australia

14:00 – 14:10 PA 15

Dielectric properties of liquefied dimethyl ether + ethanol + water mixtures at 303.2 K

Taka-aki Hoshina^{*1}, Shohei Koizumi¹, Masaki Okada¹, Tomoya Tsuji², Toshihiko Hiaki¹

¹ Nihon University, Japan

² Universiti Teknologi Malaysia (UTM) Kuala Lumpur, Malaysia

14:10 – 14:20 PA 16

Prediction of thermal conductivities for liquid mixture using ASOG-ThermConduct model

Katsumi Tochigi^{*1}, Hiroyuki Matsuda¹, Kiyofumi Kurihara¹, Tomoya Tsuji², Toshitaka Funazukuri³, V. K. Rattan⁴

¹ Nihon University, Japan

² Universiti Teknologi Malaysia, Malaysia

³ Chuo University, Japan

⁴ GNA University, India

14:20 – 14:40 PA 12 – PA 16 Questions

13:30 – 14:40 Poster Session with Flash Talk Room B

Chair: Hirohisa Uchida (Kanazawa University, Japan) and Prof. Makoto Akizuki (University of Tokyo, Japan)

13:30 – 13:40 PB 12

Cation effects on physical properties of acetate-based ionic liquids

Takashi Makino^{*1}, Tatsuya Umecky², Mitsuhiro Kanakubo¹

¹ National Institute of Advanced Industrial Science and Technology, Japan

² Saga University, Japan

13:40 – 13:50 PB 13

Thermodynamic stabilities of clathrate hydrates including tetrahydrofuran and quaternary onium salts

Takeshi Sugahara^{*1}, Hironobu Machida²

¹ Osaka University, Japan

² Panasonic Corporation, Japan

13:50 – 14:00 PB 14

Measurements of diffusion coefficient for triolein in various pressurized fluids with different viscosities

Guoxiao Cai¹, Wataru Katsumata¹, Idzumi Okajima¹, Takeshi Sako¹, Toshitaka Funazukuri², Chang Yi Kong^{*1}

¹ Shizuoka University, Japan

² Chuo University, Japan

14:00 – 14:10 PB 15

Molecular dynamics study on nucleation process for supersaturated ZnO solutions in hydrothermal conditions

Tetsuo Honma^{*1}, Kouichiro Kurosawa¹, Tasuku Murata^{1,2}, Takafumi Sato²

¹ National Institute of Technology (KOSEN), Hachinohe College, Japan

² Utsunomiya University, Japan

14:10 – 14:20 PB 16

Correlation of solubilities in mixed-solvents with local-composition-regular solution theory

Jia Lin Lee¹, Gun Hean Chong^{*,1}, Asami Kanno², Masaki Ota², Haixin Guo², Richard Lee Smith, Jr.²

¹ Universiti Putra Malaysia, Malaysia ² Tohoku University, Japan

14:20 – 14:40

PB 12 – PB 16 Questions

14:50 – 15:10

Closing Remarks and Student Presentation Award

Prof. Yoshiyuki Sato (Tohoku Institute of Technology, Japan)

Dr. Mitsuhiro Kanakubo (National Institute of Advanced Industrial Science and Technology, Japan)

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