## Technical Program

### September 5, 2018 (Wednesday)

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<th>Time</th>
<th>Session/Workshop</th>
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<td>8:30 – 8:40</td>
<td>Opening Remarks</td>
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<td></td>
<td>Prof. Kiyofumi Kurihara (Nihon University, Japan)</td>
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<tr>
<td>8:40 – 9:20</td>
<td>Plenary Lecture PL 01</td>
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<td></td>
<td>Chair: Prof. Yoshio Iwai (Kyushu University, Japan)</td>
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<tr>
<td></td>
<td><strong>Molecular design and prediction of structure and physical properties of complex chemical systems of importance to the oil and gas industry</strong></td>
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<tr>
<td></td>
<td>Ioannis G. Economou*</td>
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<td></td>
<td>Texas A&amp;M University at Qatar, Qatar</td>
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<tr>
<td>9:20 – 10:30</td>
<td>Session I</td>
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<td></td>
<td>Chair: Dr. Z. Nevin Gerek (AVEVA Group plc., USA) and Prof. Katsumi Tochigi (Nihon University, Japan)</td>
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<tr>
<td>9:20 – 10:00</td>
<td>Keynote Lecture KL 01</td>
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<tr>
<td></td>
<td>Examining the self-assembly of stratum corneum lipid mixtures</td>
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<tr>
<td></td>
<td>Tim Moore, Donna Xia, Anne Leonhard, Chris Iacovella, Clare McCabe*</td>
</tr>
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<td></td>
<td>Vanderbilt University, USA</td>
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<tr>
<td>10:00 – 10:30</td>
<td>Invited Lecture IL 01</td>
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<td></td>
<td>Correlation of phase equilibria by new activity coefficient model</td>
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<td></td>
<td>Yoshio Iwai*, Ryosuke Seki, Yoshihiro Tanaka</td>
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<td></td>
<td>Kyushu University, Japan</td>
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<tr>
<td>10:30 – 10:50</td>
<td>Coffee Break</td>
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**MTMS ’18, Narashino, Japan, September 4 – 7, 2018**
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<td>10:50 – 12:20</td>
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<td>12:00 – 12:40</td>
<td>OP 01</td>
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<tr>
<td>13:50 – 15:40</td>
<td>Session III</td>
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### Session I

**Chair:** Prof. Richard L. Smith (Tohoku University, Japan) and Prof. Tetsuo Honma (National Institute of Technology, Hachinohe College, Japan)

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<td><strong>Keynote Lecture KL 02</strong></td>
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<td><strong>OP 01</strong></td>
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<tr>
<td>13:50 – 15:40</td>
<td><strong>Session III</strong></td>
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### Keynote Lecture KL 02

**Computational screening of soft materials systems with application to nano-lubrication systems**

Andrew Z. Summers, Christopher R. Iacovella, Clare McCabe, Peter T. Cummings*
Vanderbilt University, USA

### Invited Lecture IL 02

**Multiscale modeling and simulations of protein adsorption at interfaces**

Jian Zhou*
South China University of Technology, P. R. China

### 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**

Tomohiko Yamaguchi*, Satoru Momoki
Nagasaki University, Japan

### Session II

**Chair:** Prof. Edward Maginn (University of Notre Dame) and Prof. Taka-aki Hoshina (Nihon University, Japan)

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<th>Time</th>
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<td>10:50 – 11:30</td>
<td><strong>Keynote Lecture KL 03</strong></td>
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<td>13:50 – 14:30</td>
<td><strong>Keynote Lecture KL 03</strong></td>
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<td>13:50 – 14:30</td>
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<td>14:30 – 15:00</td>
<td><strong>OP 03</strong></td>
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<td>15:00 – 15:20</td>
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### Keynote Lecture KL 03

**Current status and challenges in electrolyte thermodynamics**

Georgios M. Kontogeorgis*
Technical University of Denmark, Denmark

### 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

### OP 03

**Effective charge of ionic liquid determined through MD/DFT self-consistent scheme**

Ryosuke Ishizuka*, Nobuyuki Matubayasi1,2

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 Suzuki¹, Junichi Sakabe¹, Toshitaka Funazukuri¹*,¹, Chang Yi Kong²
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, Edward J. Maginn*
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 Mase¹,², Yusuke Shimoyama*
¹ Idemitsu Kosan Co., Ltd., Japan ² Tokyo Institute of Technology, Japan

18:00 – 20:00 Dinner
September 6, 2018 (Thursday)

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<tr>
<th>8:30 – 9:00</th>
<th>Session V</th>
<th>Chair: Prof. Takeshi Sugahara (Osaka University, Japan) and Dr. Seiya Hirohama (AVEVA Group plc., USA)</th>
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<tr>
<th>8:30 – 9:00</th>
<th>Invited Lecture IL 04</th>
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<tr>
<td>Challenges and solutions for next generation process simulators</td>
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<tr>
<td>Z. Nevin Gerek Ince*, Seiya Hirohama, David Bluck</td>
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<tr>
<td>AVEVA Group plc., USA</td>
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<th>9:00 – 10:00</th>
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<td>Flash Presentation for Young Researchers</td>
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<tr>
<td>Chair: Prof. Takeshi Sugahara (Osaka University, Japan) and Dr. Seiya Hirohama (AVEVA Group plc., USA)</td>
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<th>9:00 – 9:10</th>
<th>FP 01</th>
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<tr>
<td>Phase behavior and phase equilibria for the polydisperse polyethylene + ethylene + hexane system at high pressures and temperature: Experiments and Correlations</td>
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<tr>
<td>Rizqy Romadhona Ginting, Daichi Nakata, Kazunori Himemura, Ikuo Ushiki, Shin-ichi Kihara, Shigeki Takishima*</td>
<td></td>
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<tr>
<td>Hiroshima University, Japan</td>
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<tr>
<th>9:10 – 9:20</th>
<th>FP 02</th>
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<tr>
<td>Measurement of binary diffusion coefficient for Cr(acac)$_3$ in high temperature region of supercritical carbon dioxide</td>
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<tr>
<td>Minoru Yamamoto¹, Sakabe Junichi¹, Toshitaka Funazukuri*¹, Chang Yi Kong²</td>
<td></td>
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<tr>
<td>¹ Chuo University, Japan  ² Shizuoka University, Japan</td>
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<tr>
<th>9:20 – 9:30</th>
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<tr>
<td>Increased biocatalytic activity in CO$_2$-expanded bio-based liquids</td>
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<tr>
<td>Hai Nam Hoang¹, Emanuel Granero-Fernandez², Shinjiro Yamada¹, Shuichi Mori³, Hiroyuki Kagechika³, Yaocihuatl Medina-Gonzalez², Tomoko Matsuda*¹</td>
<td></td>
</tr>
<tr>
<td>¹ Tokyo Institute of Technology, Japan  ² Université de Toulouse, France  ³ Tokyo Medical and Dental University, Japan</td>
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<tr>
<th>9:30 – 9:40</th>
<th>FP 04</th>
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<tr>
<td>Density, viscosity, and CO$_2$/CH$_4$ solubility selectivity in protic and aprotic ionic liquids</td>
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<tr>
<td>Masaki Watanabe¹, Daisuke Kodama*¹, Takashi Makino², Mitsuhiro Kanakubo²</td>
<td></td>
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<tr>
<td>¹ Nihon University, Japan  ² National Institute of Advanced Industrial Science and Technology (AIST), Japan</td>
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<tr>
<th>9:40 – 9:50</th>
<th>FP 05</th>
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<tr>
<td>Thermodynamic property measurements and modeling for chemical hydrogen storage mediums</td>
<td></td>
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</table>
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

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<tr>
<td>8:30 – 10:40</td>
<td>Chair: Prof. Daisuke Kodama (Nihon University, Japan) and Prof. Mitsuru Sasaki (Kumamoto University, Japan)</td>
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#### 8:30 – 9:10  Keynote Lecture KL 05
**Capturing impurities from oil and gas using deep eutectic solvents**
Samah E.E Warrag¹,², 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 Ashizuka¹, Kosuke Goto¹, Takahiko Yamashita¹, Tetsuo Honma²,
Mitsuru Sasaki³
¹ Nagasaki University, Japan
² National Institute of Technology, Hachinohe College, Japan
³ Kumamoto University, Japan

#### 9:40 – 10:00  OP 09
**CO\(_2\) solubility and phase behavior in phase separation solvent at high pressure**
Andrzej-Alexander Litwinowicz¹, Takashi Makino¹, Yuki Kohno¹, Hiroshi Machida², Koyo Norinaga², 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 CO\(_2\) 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 Sharifi¹, John A. Ripmeester¹,³, Peter Englezos¹
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
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<td>11:00 – 13:00</td>
<td>Session VIII</td>
<td>Chair: Prof. Ikuo Ushiki (Hiroshima University, Japan) and Dr. Takashi Makino (AIST, Japan)</td>
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<td>11:00 – 11:30</td>
<td>Invited Lecture IL 06</td>
<td>Development of fast continuous supercritical CO₂ extraction/separation process using micromixer</td>
<td>Tatsuya Fujii(^*); Y. Matsuo(^1), S. Kawasaki(^1)</td>
<td>National Institute of Advanced Industrial Science and Technology (AIST), Japan.</td>
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<td>11:30 – 12:00</td>
<td>Invited Lecture IL 07</td>
<td>Materials informatics for designing functional liquids</td>
<td>Hirotoshi Mori(^*)</td>
<td>Ochanomizu University, Japan</td>
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<td>12:00 – 12:20</td>
<td>OP 12</td>
<td>Development of simulation technology for cement manufacturing process</td>
<td>Morihisa Yokota(^*), Tatsurou Izumi, Takeshi Suemasu</td>
<td>UBE Industries, Ltd., Japan</td>
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<td>12:20 – 12:40</td>
<td>OP 13</td>
<td>A prediction method of vapor pressure from boiling point data</td>
<td>Shuzo Ohe(^*)</td>
<td>Tokyo University of Science, Japan</td>
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<td>12:40 – 13:00</td>
<td>OP 14</td>
<td>Pressure dependency of azeotropic point for binary system methanol + dimethyl carbonate</td>
<td>Hiroyuki Matsuda(^*), M. Negishi, S. Iino, K. Kurihara, K. Tochigi, K. Ochi</td>
<td>Nihon University, Japan</td>
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<td>13:00 – 13:10</td>
<td>Closing Remarks and Student Poster Award</td>
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<td>Prof. Kiyofumi Kurihara (Nihon University, Japan)</td>
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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 trimethylether + 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 Hashimoto¹², Hiroyuki Ozeki¹, Sanehiro Muromachi*¹²
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 Research Institute of Innovative Technology for the Earth, Japan
³ Universiti Teknologi Malaysia, Malaysia

PP 06
Interfacial Tension of CO₂/EtOH/PS ternary system
Hiroaki Matsukawa*¹, Yuichiro Shimada², Masakazu Naya¹, Atsushi Shono¹, Katsuto Otake¹
¹ Tokyo University of Science, Japan
² Nagoya University, Japan
Measurement and correlation of vapor – liquid distribution coefficients of flavonoids in supercritical carbon dioxide – ethanol – water systems
Soma Sato*, Masaki Ota, Yoshiyuki Sato, Richard L. Smith, Jr., Hiroshi Inomata
Tohoku University, Japan

PP 08
Memory effect and hydrate reformation from TBAB aqueous solution - SEM observation
Hironobu Machida*,1, Hiroyasu Masunaga2, Takeshi Sugahara3, Izumi Hirasawa4
1 Panasonic Corporation, Japan
2 Japan Synchrotron Radiation Research Institute, SPring-8, Japan
3 Osaka University, Japan
4 Waseda University, Japan

PP 09
PVT relationships of methyltrimethoxysilane and tetramethyl orthosilicate
Hiroyuki Suzuki1, Hiroaki Matsukawa1, Yuichiro Shimada2, Masakazu Naya1, Atsushi Shono1, Taka-aki Hoshina3, Tomoya Tsuji4, Katsuto Otake*,1
1 Tokyo University of Science, Japan
2 Nagoya University, Japan
3 Nihon University, Japan
4 University Technology Malaysia, Malaysia

PP 10
A generalized model for predicting adsorption equilibria of various VOCs on activated carbon in supercritical carbon dioxide
Ikuo Ushiki*,1, Yoshiyuki Sato2, Yasuyuki Ito3, Shigeki Takishima1, Hiroshi Inomata2
1 Hiroshima University, Japan
2 Tohoku University, Japan
3 DAI-DAN Co., Ltd., Japan

PP 11
Phase equilibrium relations of semiclathrate hydrates based on tetra-n-butylphosphonium formate, acetate, propionate and lactate
Jin Shimada1, Masami Shimada1, Takeshi Sugahara2, Katsuhiko Tsunashima*,1
1 National Institute of Technology, Wakayama College, Japan
2 Osaka University, Japan

PP 12
Representation of solubilities of phenylthioanthraquinone in supercritical carbon dioxide using Hansen solubility parameter
Kazuhiro Tamura*, Takuya Fukamizu
Kanazawa University, Japan

PP 13
Thermodynamic stabilities of tetra-n-butylphosphonium + gas semiclathrate hydrate systems
Masami Shimada1, Takeshi Sugahara2, Katsuhiko Tsunashima*,1
1 National Institute of Technology, Wakayama College, Japan
2 Osaka University, Japan

PP 14
Phase equilibrium measurement of semicloathrate hydrates by differential scanning calorimetry
Takeshi Sugahara*,1, Hironobu Machida2
1 Osaka University, Japan 2 Panasonic Corporation, Japan

PP 15
Densities for CO2 / C6H12, C6H11CH3 and C2H5C6H5 systems
Ken Kuwabara1, Hiroaki Matsukawa1, Yuichiro Shimada2, Masakazu Naya1, Atsushi Shono1, Tomoya Tsuji3, Katsuto Otake*1
1 Tokyo University of Science, Japan 2 Nagoya University, Japan 3 University Technology Malaysia, Malaysia

PP 16
Development a new rolling ball viscometer for CO2 expanded liquids
Yoshiyuki Sato*, Hiroki Baba, Chisato Yoneyama, Hiroshi Inomata
Tohoku University, Japan

PP 17
Measurement and correlation of the SO2/PEGDME system with activity coefficient models
Ryoichi Shinozuka1, Hiroaki Matsukawa1, Yuichiro Shimada2, Masakazu Naya1, Atsushi Shono1, Tomoya Tsuji3, Katsuto Otake*1
1 Tokyo University of Science, Japan 2 Nagoya University, Japan 3 University Technology Malaysia, Malaysia

PP 18
Continuous reactive crystallization of transparent oxide semiconductor CuAlO2 in supercritical water
Takafumi Ueno, Toshiyuki Sato*, Toshihiko Hiaki
Nihon University, Japan

PP 19
Effect of solid co-solvent addition on the glass transition temperature of pharmaceutical excipients under high pressure carbon dioxide
Shiho Isono1, Hiroaki Matsukawa1, Yuichiro Shimada2, Masakazu Naya1, Atsushi Shono1, Katsuto Otake*1
1 Tokyo University of Science, Japan 2 Nagoya University, Japan

PP 20
Vapor pressure and liquid density of 1-butyl-3-methylimidazolium tetrafluoroborate + ammonia mixtures
Daisuke Tomida*, Yuki Tani, Kun Qiao, Chiaki Yokoyama
Tohoku University, Japan

PP 21
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
Tohoku University, Japan

**PP 22**
Measurement and modeling of infinite dilution activity coefficients for organic compounds in ionic liquid mixtures ([Bmim]Cl₀.₅₀[Tf₂N]₀.₅₀)
Tomoka Shida, Yuya Hiraga, Takuya Sugiyama, Yoshiyuki Sato, Masaru Watanabe, Richard L. Smith, Jr.*
Tohoku University, Japan

**PP 23**
Novel method for Screening hypertension suppressing substance from soybean milk protein
Ryunosuke Mitani*, Kenji Mishima, Tanjina Sharmin, Taku Michael Aida, Miyuki Nakamura
Fukuoka University, Japan

**PP 24**
Screening of phase separation solvent for CO₂ capture by COSMO-RS
Hiroshi Machida*, Mana Nakaoka, Tran Viet Bao Khuyen, Koyo Norinaga
Nagoya University, Japan

**PP 25**
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*
Tohoku University, Japan

**PP 26**
Dielectric properties of liquefied propane + alcohol mixtures at 303.2 K
Taka-aki Hoshina*¹, Yusuke Koshiba¹, Masaki Okada¹, Tomoya Tsuji², Toshihiko Hiaki³
¹ Nihon University, Japan ² Universiti Teknologi Malaysia, Malaysia

**PP 27**
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*
Kanazawa University

**PP 28**
Measurement of non-ideality of hansen solubility parameter for solvent mixture using physical properties
Takuya Tamura*, Hideki Yamamoto
Kansai University, Japan

**PP 29**
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
Designing ionic liquids for efficient CO$_2$ capture: A materials informatics study

Nahoko Kuroki, Hiroshi Mori*

Ochanomizu University, Japan

Density, viscosity, and CO$_2$ solubility in deep eutectic solvents composed of quaternary ammonium salt and ethylene glycol

Ayaka Taniguchi$^1$, Daisuke Kodama$^1$*, Masaki Watanabe$^1$, Takashi Makino$^2$, Mitsuhiro Kanakubo$^2$

$^1$ Nihon University, Japan
$^2$ National Institute of Advanced Industrial Science and Technology (AIST), Japan

CO$_2$ absorption and physical properties of tributylcytolphosphonium benzotriazolate

Takashi Makino$^1$*, Katsuhiko Tsunashima$^2$, Mitsuhiro Kanakubo$^1$

$^1$ National Institute of Advanced Industrial Science and Technology (AIST), Japan
$^2$ National Institute of Technology, Wakayama College, Japan

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

Yuva Murakami, Yusuke Torita, Yusuke Shimoyama*

Tokyo Institute of Technology, Japan

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

Yusuke Tsuchida$^1$, Masahiko Matsumiya$^1$*, Katsuhiko Tsunashima$^2$

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