

# Technical Program

August 5 (Wed)

8:30-8:40 **Opening Remarks**

8:40-9:20 **[Plenary Lecture 1]**

Chair: Prof. Katsumi Tochigi (Nihon Univ., Japan)

**Understanding the self-assembly and phase behavior of skin lipids**

Clare McCabe (Vanderbilt Univ., USA)

**[Session I, 9:20-10:30]**

Chair: Prof. Zhiping Liu (Beijing Univ. Chem. Tech., China), Dr. Mitsuhiro Kanakubo (AIST, Japan)

9:20-10:00 **[Keynote Lecture 1]**

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

José Nuno Canongia Lopes\*<sup>1,2</sup>, Karina Shimizu<sup>1</sup>, Carlos E. S. Bernardes<sup>1</sup> (<sup>1</sup>Univ. de Lisboa, Portugal, <sup>2</sup>Univ. Nova de Lisboa, Portugal )

10:00-10:30 **[Invited Lecture 1]**

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

Seiji Tsuzuki (AIST, Japan)

**10:30-10:50 Coffee Break**

**[Session II, 10:50-12:40]**

Chair: Prof. José Nuno Canongia Lopes (Univ. de Lisboa, Portugal), Dr. Seiji Tsuzuki (AIST, Japan)

10:50-11:20 **[Invited Lecture 2]**

**Z-bond and molecular simulation of ionic liquids**

Suojiang Zhang\*, Xiaomin Liu (Chinese Acad. Sci., China)

11:20-11:40 **[OP 1]**

**Energetic contributions from the cation and anion to the stability of carbon dioxide dissolved in imidazolium-based ionic liquids**

Ryosuke Ishizuka\*, Nobuyuki Matubayasi (Osaka Univ., Japan)

11:40-12:00 **[OP 2]**

**Measurement and correlation of infinite dilution partition coefficients for *o*, *m*, *p*-cresol and related benzene derivatives in [bmim][Tf<sub>2</sub>N]-CO<sub>2</sub> biphasic system**

Yuya Hiraga\*, Yoshiyuki Sato, Masaru Watanabe, Taku M. Aida, Richard L. Smith, Jr. (Tohoku Univ., Japan)

12:00-12:40 **[Keynote Lecture 2]**

**Integrated experimental and computational studies of energy-relevant interfaces**

Peter Cummings (Vanderbilt Univ., USA)

**12:40-13:50 Lunch**

**[Session III, 13:50-15:20]**

Chair: Prof. Gabriele Sadowski (TU Dortmund, Germany), Prof. Daisuke Kodama (Nihon Univ., Japan)

13:50-14:30 **[Keynote Lecture 3]**

**Ionic liquids versus deep eutectic solvents**

Francisco, M.<sup>1</sup>, Bruinhorst, A. van den<sup>1</sup>, Zubeir, L.F.<sup>1</sup>, Peters, C.J.<sup>1,2</sup>, Kroon, M.C.<sup>1</sup> (<sup>1</sup>Eindhoven Univ. Tech., The Netherlands, <sup>2</sup>Petro. Ins., UAE)

14:30-15:00 **[Invited Lecture 3]**

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

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

15:00-15:20 **[OP 3]**

**Phase transition solvent for CO<sub>2</sub> capture process**

Hiroshi Machida, Takashi Tomikawa, Hirotochi Horizoe (Nagoya Univ., Japan)

**15:20-15:40 Coffee Break**

**[Session IV, 15:40-17:20]**

Chair: Prof. Jeong Won Kang (Korea Univ., Korea), Prof. Hiroyuki Matsuda (Nihon Univ., Japan)

15:40-16:20 **[Keynote Lecture 4]**

**Equations of state in three centuries – Perspectives and future challenges**

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

16:20-16:50 **[Invited Lecture 4]**

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

Nevin Gerek Ince<sup>1\*</sup>, Gang (Gary) Xu<sup>1</sup>, Seiya Hirohama<sup>2</sup>, Prasad Narasimhan<sup>3</sup> (<sup>1</sup>Schneider Electric, Lake Forest, USA, <sup>2</sup>Schneider Electric, Japan, <sup>3</sup>Schneider Electric, Houston, USA)

16:50-17:20 **[Invited Lecture 5]**

**Modeling the solubility of co-crystals and hydrates**

Gabriele Sadowski, Linda Lange (TU Dortmund, Germany)

**[Session V, 17:20-19:00]**

Chair: Prof. Jae-Jin Shim (Yeungnam Univ., Korea), Prof. Yusuke Shimoyama (Tokyo Inst. Tech., Japan)

17:20-18:00 **[Keynote Lecture 5]**

**New modified UNIFAC parameters using critically evaluated phase equilibrium data**

Jeong Won Kang<sup>\*1</sup>, Vladimr Diky<sup>2</sup>, Michael Frenkel<sup>2</sup> (<sup>1</sup>Korea Univ., Korea, <sup>2</sup>NIST, USA)

18:00-18:30 **[Invited Lecture 6]**

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

Liu Zhiping<sup>\*</sup>, Du Xiaona (Beijing Univ. Chem. Tech., China)

18:30-19:00 **[Invited Lecture 7]**

**Prediction of phase transition of FCC and HCP hard-sphere crystals via free volume approach**

Sang Kyu Kwak<sup>\*</sup>, Dae Yeon Hwang, Jeong Hyeon Lee (UNIST, Korea)

**19:00- Dinner**

## **August 6 (Thu)**

### **[Session VI, 8:30-9:40]**

Chair: Prof. Md. Zaidul Islam Sarker (Int. Islamic Univ., Malaysia), Prof. Masashi Haruki (Hiroshima Univ., Japan)

8:30-9:00 **[Invited Lecture 8]**

#### **Controlled living polymerization in supercritical carbon dioxide**

Jae-Jin Shim<sup>\*</sup>, Van Hoa Nguyen, Naoshad Islam, Kaikai Chen (Yeungnam Univ., Korea)

9:00-9:20 **[OP 4]**

#### **Recycling of carbon fiber reinforced plastic using supercritical alcohol**

Idzumi Okajima<sup>\*</sup>, Yoshinobu Shimamura, Takeshi Sako (Shizuoka Univ., Japan)

9:20-9:40 **[OP 5]**

#### **Microencapsulation of phenylalanine with pH-responsive polymer for controlled release of drug by pressure-induced phase separation of CO<sub>2</sub> solution**

Kenji Mishima<sup>\*1</sup>, Shota Ito<sup>1</sup>, Ryo Kawakami, Tanjina Sharmin<sup>1</sup>, Hazuki Nerome<sup>1</sup>, Hiroki Kusakabe<sup>1</sup>, Saori Hirayama<sup>1</sup>, Takafumi Kato<sup>1</sup>, Makoto Misumi<sup>1</sup>, Tadashi Suetsugu<sup>1</sup>, Hideaki Orii<sup>1</sup>, Keiichi Irie<sup>1</sup>, Kazunori Sano<sup>1</sup>, Kenichi Mishima<sup>1</sup>, Takunori Harada<sup>2</sup> (<sup>1</sup>Fukuoka Univ., Japan, <sup>2</sup>Oita Univ., Japan)

**9:40-10:00 Coffee Break**

**10:00-12:00 Poster Presentations**

**12:00-13:20 Lunch**

**13:20-13:30 Group Photo**

**13:30- Excursion**

**19:00- Banquet**

## August 7 (Fri)

### [Session VII, 8:30-10:00]

Chair: Prof. Richard L. Smith, Jr. (Tohoku Univ., Japan), Dr. Takashi Makino (AIST, Japan)

#### 8:30-9:00 [Invited Lecture 9]

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

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

#### 9:00-9:20 [OP 6]

##### **Measurement of diffusion coefficient and solubility estimation for dyes in supercritical carbon dioxide by CIR method**

Toshitaka Funazukuri\*<sup>1</sup>, Taichi Yamasaki<sup>1</sup>, Minoru Taguchi<sup>1</sup>, Chang Yi Kong<sup>2</sup> (<sup>1</sup>Chuo Univ., Japan, <sup>2</sup>Shizuoka Univ., Japan)

#### 9:20-9:40 [OP 7]

##### **Development of a generalization model of VOCs adsorption equilibria on various adsorbents under supercritical carbon dioxide conditions by using the Dubinin-Astakhov equation**

Ikuo Ushiki\*<sup>1</sup>, Masaki Ota, Yoshiyuki Sato, Hiroshi Inomata (Tohoku Univ., Japan)

#### 9:40-10:00 [OP 8]

##### **Measurement and correlation of the solid-liquid-gas equilibria for carbon dioxide + drug systems: Carbon dioxide + acetylsalicylic acid (aspirin) and carbon dioxide + phenylbutazone systems**

Hirohisa Uchida\*<sup>1</sup>, Mika Natsume<sup>1</sup>, Kyohei Sano<sup>1</sup>, Yoshiyuki Kojima<sup>2</sup>, Masakuni Matsuoka<sup>2</sup> (<sup>1</sup>Shinshu Univ., Japan, <sup>2</sup>Tokyo Univ. Agr. Tech, Japan)

### 10:00-10:30 Coffee Break

### [Session VIII, 10:30-11:50]

Chair: Dr. Takafumi Aizawa (AIST, Japan), Prof. Hirohisa Uchida (Shinshu Univ., Japan)

#### 10:30-10:50 [OP 9]

##### **Thermodynamic properties prediction containing unfamiliar or big molecules based on component family method**

Hideo Nishiumi (Hosei Univ., Japan)

#### 10:50-11:10 [OP 10]

##### **Modeling ternary vapor-liquid-equilibrium (VLE) of carbon dioxide (CO<sub>2</sub>) + water + tetraethylene glycol (TEG) for the temperature range from 277K to 398 K, and the optimization of the pre-combustion CO<sub>2</sub> capture process.**

Shigeo Oba\*<sup>1</sup>, Tomoya Tsuji<sup>2</sup> (<sup>1</sup>App. Thermody. Phys. Prop., Japan, <sup>2</sup>Nihon Univ., Japan)

#### 11:10-11:30 [OP 11]

##### **A prediction method of non-ideal vapor-liquid equilibrium using cluster model**

Shuzo Ohe (Tokyo Univ. Sci., Japan)

#### 11:30-11:50 [OP 12]

##### **Solvent effects of ethyl lactate as an entrainer for the separation of the binary azeotropic mixture by extractive distillation**

Hiroyuki Matsuda<sup>\*</sup>, Koji Inaba, Hirofumi Sumida, Kiyofumi Kurihara, Katsumi Tochigi, Kenji Ochi  
(Nihon Univ., Japan)

**11:50-12:00 Commendation Ceremony of Student Poster Awards**

**12:00-12:10 Closing Remarks**

**12:10-13:10 Lunch**

## List of Poster Presentations

### PP 1

**Prediction of liquid - liquid equilibria for alkane + methanol + aromatic hydrocarbon ternary systems by using modified Wilson equation with parameters estimated from pure-component properties**

Shigetoshi Kobuchi<sup>\*</sup>, Tsuyoshi Kamiryō, Setsuko Yonezawa, Yasuhiko Arai (Yamaguchi Univ., Japan)

### PP 2

**Prediction of VOCs adsorption equilibria on various adsorbents in supercritical carbon dioxide by using pure component adsorption data**

Ikuo Ushiki<sup>\*</sup>, Masaki Ota, Yoshiyuki Sato, Hiroshi Inomata (Tohoku Univ., Japan)

### PP 3

**Study on solubility and diffusivity of ethylene in poly(methyl methacrylate-ethyl acrylate) for controlled release material**

Yoshiyuki Sato<sup>\*1</sup>, Tomohiro Ara<sup>1</sup>, Hiroshi Inomata<sup>1</sup>, Ryoichi Yamamoto<sup>2</sup>, Shigeru Haeno<sup>2</sup>, Masayoshi Johmen<sup>2</sup> (<sup>1</sup>Tohoku Univ., Japan, <sup>2</sup>Hitachi Chemical, Japan)

### PP 4

**Dynamic properties of methanol-water mixture in the temperature range up to 476.2 K and high pressure via molecular dynamics simulation**

Takumi Ono<sup>\*</sup>, Masaki Ota, Yoshiyuki Sato, Hiroshi Inomata (Tohoku Univ., Japan)

### PP 5

**Prediction of the liquid-liquid phase equilibria for the polydisperse polyethylene solutions under the high temperature and pressure conditions**

Masashi Haruki<sup>\*</sup>, Kotaro Adachi, Shohei Fujikawa, Shin-ichi Kihara, Shigeki Takishima<sup>\*</sup> (Hiroshima Univ., Japan)

### PP 6

**Experimental and simulation studies of physical foaming process using high-pressure CO<sub>2</sub>**

Ying Sun, Yumi Ueda, Hiroyuki Suganaga, Masashi Haruki, Shin-ichi Kihara, Shigeki Takishima<sup>\*</sup> (Hiroshima Univ., Japan)

### PP 7

**Preparation of nano-particle/polymer hybrid particles using supercritical fluids**

Shin-ichi Kihara<sup>\*</sup>, Yorisada Ozaki, Shotaro Ohno, Masashi Haruki, Shigeki Takishima<sup>\*</sup> (Hiroshima Univ., Japan)

### PP 8

**Densities, viscosities, and electrical conductivities of 1-ethyl-3-methylimidazolium ionic liquids with 2,4-pentandionate and 1,1,1-trifluoro-2,4-pentandionate anions**

Tatsuya Umecky<sup>\*1</sup>, Mitsutoshi Abe<sup>1</sup>, Toshiyuki Takamuku<sup>1</sup>, Takashi Makino<sup>2</sup>, Mitsuhiro Kanakubo<sup>2</sup> (<sup>1</sup>Saga Univ., Japan, <sup>2</sup>AIST, Japan)

### PP 9

**Measurement of vapor pressure using gas chromatograph method**

Jun Mase, Shinji Miyamoto (Idemitsu Kosan, Japan)

### PP 10

**Measurement of vapor-liquid equilibria in the region of extremely dilute composition for four alcohol + water systems**

Katsumi Tochigi<sup>\*1</sup>, Masahiko Ito<sup>1</sup>, Hiromasa Taguchi<sup>2</sup>, Hiroyuki Matsuda<sup>1</sup>, Kiyofumi Kurihara<sup>1</sup>  
(<sup>1</sup>Nihon Univ., Japan, <sup>2</sup>PreFEED, Japan)

**PP 11**

**Determination and correlation of heat of mixing of the binary carbon dioxide + *tert*-butyl methyl ether (TBME) system at temperatures from (298.15 to 308.15) K and pressures from (5.0 to 7.0) MPa**

Tomohiro Kobayashi, Tomoaki Kasai, Kiyofumi Kurihara<sup>\*</sup>, Hiroyuki Matsuda, Katsumi Tochigi (Nihon Univ., Japan)

**PP 12**

**Liquid-liquid equilibria of the mixture water + alkane + non-ionic surfactant**

Yuki Nakazato, Rei Tsuchiya, Hiroyuki Matsuda<sup>\*</sup>, Kiyofumi Kurihara, Katsumi Tochigi (Nihon Univ., Japan)

**PP 13**

**CO<sub>2</sub> chemisorption behavior of 1-butyl-3-methylimidazolium acetate in the mixtures with 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)amide**

Mitsuhiro Kanakubo<sup>\*1</sup>, Takashi Makino<sup>1</sup>, Tatsuya Umecky<sup>2</sup>, Masato Sakurai<sup>3</sup> (<sup>1</sup>AIST, Japan, <sup>2</sup>Saga Univ., Japan, <sup>3</sup>Japan Aerospace Exploration Agency, Japan)

**PP 14**

**CO<sub>2</sub> absorption and physical properties of tetrabutylphosphonium prolinat**

Takashi Makino<sup>\*1</sup>, Mitsuhiro Kanakubo<sup>\*1</sup>, Shohei Kasahara<sup>2</sup>, Eiji Kamio<sup>2</sup>, Hiromitsu Takaba<sup>3</sup>, Hideto Matsuyama<sup>1</sup> (<sup>1</sup>AIST, Japan, <sup>2</sup>Kobe Univ., Japan, <sup>3</sup>Kogakuin Univ., Japan)

**PP 15**

**Fabrication of nano-structured titania aerogels using sol – gel reaction and drying in supercritical carbon dioxide**

Motohiro Kinoshita, Yusuke Shimoyama (Tokyo Inst. Tech., Japan)

**PP 16**

**Mass transfer analysis on supercritical carbon dioxide drying**

Nattanai Kunanusont, Motohiro Kinoshita, Yusuke Shimoyama (Tokyo Inst. Tech., Japan)

**PP 17**

**Microfluidic extraction of emulsion using supercritical carbon dioxide for fabrication of nanoparticle suspension in aqueous solution**

Yuya Murakami, Yusuke Shimoyama<sup>\*</sup> (Tokyo Inst. Tech., Japan)

**PP 18**

**A molecular modeling study of carbazole-based organic polycyclic compounds for hydrogen storage applications**

Byeong Soo Shin<sup>1</sup>, Sang Kyu Kwak<sup>\*2</sup>, Jeong Won Kang<sup>\*1</sup> (<sup>1</sup>Korea Univ., Korea, <sup>2</sup>UNIST, Korea)

**PP 19**

**Molecular simulation study on variation of OH-1 crystal growth habit**

In Young Choi<sup>1</sup>, Woo Sik Kim<sup>2</sup>, Jeong Won Kang<sup>\*1</sup> (<sup>1</sup>Korea Univ., Korea, <sup>2</sup>Kyung Hee Univ., Korea)

**PP 20**

**Immobilization of Pt nanoparticles inside the pores of metal-organic framework using supercritical carbon dioxide**

Kiyoshi Matsuyama<sup>\*1</sup>, Momoe Motomura<sup>1</sup>, Shiori Masuda<sup>1</sup>, Muneharu Kuboyama<sup>1</sup>, Tetsuya Okuyama<sup>1</sup>, Hiroyuki Moto<sup>2</sup> (<sup>1</sup>Kurume Nat. College Tech., Japan, <sup>2</sup>Toyohashi Univ. Tech., Japan)

**PP 21**

**New recycling process of plastic containers and packaging**

Nozomi Takenaka<sup>1</sup>, Naoto Oda<sup>1</sup>, Aya Tominaga<sup>1</sup>, Hiroshi Sekiguchi<sup>1</sup>, Ryoko Nakano<sup>1</sup>, Shigeru Yao<sup>1</sup>, Eiichi Takatori<sup>2</sup> (<sup>1</sup>Fukuoka Univ., Japan, <sup>2</sup>TOSOH A&R Center, Japan)

**PP 22**

**The spherical PE particulate species dependence of thermal rheological fluid effect**

Yuri Kanazawa, Yusuke Hasebe, Kouki Hirakawa, Ryoko Nakano, Hiroshi Sekiguchi, Shigeru Yao (Fukuoka Univ., Japan)

**PP 23**

**The supramolecular interaction between side chain crystalline block co-polymer and poly(tetra fluor ethylene) and chemical surface modification**

Hideaki Obuchi, Ryoko Nakano, Ai Maeda, Fumiharu Yamasaki, Hiroshi Sekiguchi, Shigeru Yao\* (Fukuoka Univ., Japan)

**PP 24**

**Numerical simulations of droplet penetration into glass beds by lattice Boltzmann method**

Yosuke Matsukuma\*, Yuki Kubokawa, Hiroki Uchiyama (Fukuoka Univ., Japan)

**PP 25**

**A fluorescence quenching study for interaction of apigenin to bovine serum albumin**

Shota Ito<sup>1</sup>, Kenji Mishima<sup>\*1</sup>, Hilyatuz Zahroh<sup>2</sup>, Ryo Kawakami<sup>1</sup>, Tanjina Sharmin<sup>1</sup>, Hazuki Nerome<sup>1</sup>, Masashi Fujizono<sup>1</sup>, Yuuki Eto<sup>1</sup>, Takuya Nakashima<sup>1</sup>, Takafumi Kato<sup>1</sup>, Makoto Misumi<sup>1</sup>, Tadashi Suetsugu<sup>1</sup>, Hideaki Orii<sup>1</sup>, Keiichi Irie<sup>1</sup>, Kazunori Sano<sup>1</sup>, Kenichi Mishima<sup>1</sup>, Takunori Harada<sup>3</sup>, Yusraini Dian Inayati Siregar<sup>2</sup>, Ahmad Marup<sup>2</sup>, Lily Surayya Eka Putri<sup>2</sup>, Agus Salim<sup>2</sup> (<sup>1</sup>Fukuoka Univ., Japan, <sup>2</sup>Syarif Hidayatullah State Islamic Univ. (UIN), Indonesia, <sup>3</sup>Oita Univ., Japan)

**PP 26**

**Solubility of baicalein in supercritical carbon dioxide**

Kenji Mishima<sup>\*1</sup>, Yuuta Saeki<sup>1</sup>, Yusuke Tobana<sup>1</sup>, Shota Ito<sup>1</sup>, Ryo Kawakami, Tanjina Sharmin<sup>1</sup>, Hazuki Nerome<sup>1</sup>, Takafumi Kato<sup>1</sup>, Makoto Misumi<sup>1</sup>, Tadashi Suetsugu<sup>1</sup>, Hideaki Orii<sup>1</sup>, Keiichi Irie<sup>1</sup>, Kazunori Sano<sup>1</sup>, Kenichi Mishima<sup>1</sup>, Takunori Harada<sup>2</sup> (<sup>1</sup>Fukuoka Univ., <sup>2</sup>Oita Univ.)

**PP 27**

**Solubility of resveratrol in supercritical carbon dioxide**

Hirofumi Kawamura<sup>1,2</sup>, Kenji Mishima<sup>\*1,2</sup>, Shota Ito<sup>1</sup>, Ryo Kawakami, Tanjina Sharmin<sup>1,2</sup>, Hazuki Nerome<sup>1,2</sup>, Ryouhei Esaki<sup>1</sup>, Shion Wakiyama<sup>1</sup>, Takafumi Kato<sup>1</sup>, Makoto Misumi<sup>1</sup>, Tadashi Suetsugu<sup>1</sup>, Hideaki Orii<sup>1</sup>, Keiichi Irie<sup>1</sup>, Kazunori Sano<sup>1</sup>, Kenichi Mishima<sup>1</sup>, Takunori Harada<sup>3</sup> (<sup>1</sup>Fukuoka Univ., Japan, <sup>2</sup>San-Ei Gen F.F.I., Inc., <sup>3</sup>Oita Univ., Japan)

**PP 28**

**Measurement and correlation of diffusion coefficients of metal complex in supercritical and liquid states**

Chang Yi Kong<sup>\*1</sup>, Yoshiki Yakumaru<sup>1</sup>, Toshitaka Funazukuri<sup>2</sup> (<sup>1</sup>Shizuoka Univ., Japan, <sup>2</sup>Chuo Univ., Japan)

**PP 29**

**Volumetric and dielectric properties of dimethylether + ethanol mixtures at 293.2~313.2 K under 1 MPa**

Kazunori Sato, Taka-aki Hoshina\*, Tomoya Tsuji, Toshihiko Hiaki (Nihon Univ., Japan)



**PP 30**

**Measurement and correlation of solid-liquid equilibria for three binaries, ethanol + antipyrine, chloroform + antipyrine, and dimethyl ether + antipyrine**

Daigo Yokoi, Taka-aki Hoshina, Tomoya Tsuji\*, Toshihiko Hiaki, Daisuke Tomida, Kun Qiao, Chiaki Yokoyama (Nihon Univ., Japan, Tohoku Univ., Japan)

**PP 31**

**Estimation of melting point depression of organic compounds by high-pressure carbon dioxide**

Masaya Yanagida, Yuichiro Shimada, Atsushi Shono, Katsuto Otake\* (Tokyo Univ. Sci., Japan)

**PP 32**

**Phase behavior of CO<sub>2</sub>/tetraalkoxysilane/polymer ternary systems**

Hiroaki Matsukawa<sup>1</sup>, Yuichiro Shimada<sup>1</sup>, Atsushi Shono<sup>1</sup>, Satoshi Yoda<sup>2</sup>, Yasuo Okawa<sup>3</sup>, Katsuto Otake<sup>1\*</sup> (<sup>1</sup>Tokyo Univ. Sci., Japan, <sup>2</sup>AIST, Japan, <sup>3</sup>Showa Jyushi, Japan)

**PP 33**

**Phase behavior CO<sub>2</sub>/tetraalkoxysilane/plasticizer ternary systems**

Kazuki Sudo, Yuichiro Shimada, Daisuke Kobayashi, Atsushi Shono, Katsuto Otake\* (Tokyo Univ. Science, Japan)

**PP 34**

**Modeling of CO<sub>2</sub> solubility in tertiary amine solvent using pK<sub>a</sub>**

Hiroshi Machida<sup>\*1</sup>, Hidetaka Yamada<sup>2</sup>, Shin Yamamoto<sup>2</sup> (<sup>1</sup>Nagoya Univ., Japan, <sup>2</sup>RITE, Japan)

**PP 35**

**Compact apparatus for high-pressure vapor-liquid equilibrium, density, and viscosity measurements**

Akira Nakamura<sup>1</sup>, Yasuhiro Endo<sup>1</sup>, Daisuke Kodama<sup>\*1</sup>, Shigenobu Matsuo<sup>2</sup>, Tomohiro Sotani<sup>2</sup>, Takashi Makino<sup>3</sup>, Mitsuhiro Kanakubo<sup>3</sup> (<sup>1</sup>Nihon Univ., Japan, <sup>2</sup>Kobe Univ., Japan, <sup>3</sup>AIST, Japan)

**PP 36**

**Solubility and enthalpy data of CO<sub>2</sub> in 1-ethyl-3-methylimidazolium bis(trifluoromethane sulfonyl)amide and 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)amide**

Toshiya Sugawara<sup>1</sup>, Daisuke Kodama<sup>\*1</sup>, Takashi Makino<sup>2</sup>, Mitsuhiro Kanakubo<sup>2</sup> (<sup>1</sup>Nihon Univ., Japan, <sup>2</sup>AIST, Japan),

**PP 37**

**CO<sub>2</sub> absorption properties of imidazolium based ionic liquids using a magnetic suspension balance**

Masaki Watanabe<sup>1</sup>, Daisuke Kodama<sup>\*1</sup>, Takashi Makino<sup>2</sup>, Mitsuhiro Kanakubo<sup>2</sup> (<sup>1</sup>Nihon Univ., Japan, <sup>2</sup>AIST, Japan)

**PP 38**

**Effects of crystal polymorphism on solubility of theophylline in supercritical carbon dioxide**

Mika Natsume, Kyohei Sano, Hirohisa Uchida\* (Shinshu Univ., Japan)

**PP 39**

**A user-fitting group contribution method using TC line data accompanied with chemical groups assigned to SMILES notations**

Satoru Kato (TC Lines, Japan)

**PP 40**

**Phase behavior and solid-liquid equilibria of carboxylic acid mixtures**

Kazuhiro Tamura<sup>\*</sup>, Tsuyoshi Kasuga, Tomoyuki Nakagawa (Kanazawa Univ., Japan)

**PP 41**

**Modification of surface area parameters in CDSAP model for calculation of activity coefficients**  
Yusuke Miyazaki, Yoshio Iwai\* (Kyushu Univ., Japan)

**PP 42**

**Test of activity coefficient models by direct molecular dynamics simulation of vapor-liquid equilibria**  
Yasuhiro Tada, Yoshio Iwai\* (Kyushu Univ., Japan)

**PP 43**

**Analysis of Nafion membranes for direct methanol fuel cells treated with supercritical CO<sub>2</sub>**  
Ryuhei Hattori, Setsuko Yonezawa, Yoshio Iwai\* (Kyushu Univ., Japan)

**PP 44**

**Measurement of diffusion coefficients for Pb(acac)<sub>2</sub> in Nafion under supercritical carbon dioxide**  
Yasuo Hirayama, Setsuko Yonezawa, Yoshio Iwai\* (Kyushu Univ., Japan)

**PP 45**

**Molecular dynamics simulation of self-diffusion coefficients for Bmim TFSA + water system**  
Hidenori Higashi\*, Mikio Kumita, Takafumi Seto, Yoshio Otani (Kanazawa Univ., Japan)

**PP 46**

**Fabrication of nanocarbon by irradiating pulse laser in supercritical carbon dioxide**  
Toru Yoshikawa, Hidenori Higashi\*, Mikio Kumita, Takafumi Seto, Yoshio Otani (Kanazawa Univ., Japan)

**PP 47**

**Screening ionic liquids for dissolving cellulose by COSMO-RS**  
Yanrong Liu<sup>1</sup>, Yi Nie<sup>1</sup>, Suojiang Zhang<sup>1</sup>, Anne S. Meyer<sup>2</sup>, Kaj Thomsen<sup>2</sup>, Xiaochun Zhang<sup>1</sup>  
(<sup>1</sup>Chinese Acad. Sci., China, <sup>2</sup>Tech. Univ. Denmark, Denmark)

**PP 48**

**A new force field model with explicit hydrogen bond forms for the imidazolium-based ionic liquids**  
Feng Huo, Suojiang Zhang\* (Chinese Acad. Sci., China)

**PP 49**

**Microencapsulation of fish oil using hydroxy propyl methyl cellulose as a carrier material by spray drying**  
Fahim T.K., Zaidul I.S.M.\* (Int. Islamic Univ., Malaysia)

**PP 50**

**Ionic liquid-mediated synthesis of poly (2-hydroxyethyl methacrylate-*block*-methyl methacrylate) /Fe<sub>3</sub>O<sub>4</sub> core-shell structured nanocomposite by ATRP**  
Van Chinh Tran<sup>1</sup>, Van Hoa Nguyen<sup>1,2</sup>, Jae-Jin Shim<sup>1,\*</sup>(<sup>1</sup>Yeungnam Univ., Korea, <sup>2</sup>Nha Trang Univ., Vietnam)

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**Molecular dynamics study of the degradation of alkylsilane monolayers under shear**  
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