

# IEC

## DIVISION OF INDUSTRIAL & ENGINEERING CHEMISTRY

**Program Not Yet Complete -- Run Data Integrity Report to Identify Errors**

**Times, days, and paper numbers may not be final.**

M. A. Gonzalez, *Program Chair*

### SUNDAY MORNING

Section A

Radisson Plaza - Warwick -- Chestnut

**Celebrating the 100th Anniversary of the Journal of Industrial and Engineering Chemistry Research**

S. D. Alexandratos, *Organizer*

**9:00** — Introductory Remarks.

**9:05** —**1.** 100 Years of the journal: Industrial & Engineering Chemistry. **D. R. Paul**

**9:35** —**2.** Shared heritage of I&EC and IECR. **W. H. Flank**

**10:05** —**3.** From crystalline salts to ionic liquids and back again: In the hunt for novel separations. **R. D. Rogers**

**10:35** — Intermission.

**10:45** —**4.** Coupling reactions and separations for sustainable processes. **C. A. Eckert**, C. L. Liotta

**11:15** —**5.** Materials design for gas separation membranes. **B. D. Freeman**

**11:45** —**6.** Effect of solvent on controllability in extractive distillation. **W. L. Luyben**

Section B

Radisson Plaza - Warwick -- Crystal Ballroom

**Ionic Liquids: From Knowledge to Application**

**Gas Separations**

J. F. Brennecke, R. D. Rogers, and K. R. Seddon, *Organizers*

M. F. Costa Gomes and M. B. Shiflett, *Organizers, Presiding*

**8:30** — Introductory Remarks.

**8:35** —**7.** Ionic liquids: Promising media for gas separations. **M. F. Costa Gomes**

**8:45** —**8.** Gas solubility and related phenomena in systems with ionic liquids. **G. Maurer**

**9:05 —9.** Prediction of gas solubility in ionic liquids using COSMOtherm. **D. W. Rooney**, C. Hardacre, P. Nancarrow, J. Jacquemin, N. Ab Manan, M. F. Costa Gomes, A. A. H. Pádua

**9:25 —10.** Deep desulfurization of light refinery cuts by ionic liquid based extraction and absorption techniques. **P. Wasserscheid**, E. Kuhlmann

**9:45 —11.** Capture of CO<sub>2</sub> by using ionic liquids. **S. Zhang**, Y. Zhang, X. Lu, Q. Zhou, X. Zhang

**10:05 —12.** Carbon dioxide capture using ionic liquids. **J. F. Brennecke**, D. E. Kestel, Z. K. Lopez-castillo, J. L. Anderson, J. C. de la Fuente

**10:25 —** Intermission.

**10:40 —13.** Polymer gas separation membranes derived from and inspired by room temperature ionic liquids. J. E. Bara, T. K. Carlisle, C. J. Gabriel, **D. L. Gin**, R. D. Noble

**11:00 —14.** Tuning ionic liquids as high-capacity, reversible gas absorbers for sulphur dioxide. A. Riisager, R. W. Berg, **R. Fehrmann**

**11:20 —15.** Inverse gas chromatography (IGC) as a versatile tool for gas separation tests using ionic liquids. **T. Beyersdorff**, A. Reisinger, T. J. S. Schubert

**11:40 —16.** Phase equilibria, viscosity, and diffusivity of imidazolium ionic liquids with compressed carbon dioxide and hydrofluorocarbon gases. W. Ren, A. Aghosseini, **A. M. Scurto**

## SUNDAY AFTERNOON

Section A

Radisson Plaza - Warwick -- Chestnut

### Celebrating the 100th Anniversary of the Journal of Industrial and Engineering Chemistry Research

S. D. Alexandratos, *Organizer*

**1:30 —17.** Ion exchange resins: A retrospective from Industrial & Engineering Chemistry Research and a prospective. **S. D. Alexandratos**

**2:00 —18.** Highlighting the history of the first nanomaterial: Charcoal. **M. J. Antal Jr.**

**2:30 —19.** Design of pharmaceutical nanoparticles for drug delivery. **K. P. Johnston**, J. Engstrom, J. Tam, M. Matteucci, A. Mazuski, L. Ma, R. Williams III, T. Milner, M. Feldman

**3:00 —** Intermission.

**3:15 —20.** Functionalized magnetic nanoparticles and nanofibers for protection against chemical and biological toxicants. L. Chen, H. Zhang, L. Bromberg, K. A. Smith, G. C. Rutledge, **T. A. Hatton**

**3:45 —21.** Molecule-based modeling of heavy hydrocarbon structure and reactions. **M. T. Klein**, C. A. Bennett, Z. Hou

**4:15 —22.** Modeling of biomolecules and pharmaceuticals using PC-SAFT. **G. Sadowski**, C. Held, F. Tumakaka

Section B

Radisson Plaza - Warwick -- Crystal Ballroom

## **Ionic Liquids: From Knowledge to Application**

### **Liquid Separations**

J. F. Brennecke, R. D. Rogers, and K. R. Seddon, *Organizers*  
J. L. Anderson and P. G. Jessop, *Organizers, Presiding*

**1:30** — Introductory Remarks.

**1:35** —**23.** Separation of aromatic and aliphatic hydrocarbons with ionic liquids: A conceptual process design. **G. W. Meindersma**, A. B. de Haan

**2:00** —**24.** Liquids separations and extractions of metal ions with ionic liquids. **U. Domańska-Zelazna**

**2:25** —**25.** Tailoring ionic liquids for separation. **S. Dai**, H. Luo, D -E. Jiang

**2:50** —**26.** Ionic liquid pretreatment of lignocellulose for biofuels production. **C. Schall**, S. Varanasi, A. Dadi, T. Ponnaiyan, I. Samayam, J. Wheeler

**3:15** — Intermission.

**3:35** —**27.** Ionic liquids in RPLC, additive effects and determination. **A. Berthod**, M. J. Ruiz-Angel, S. Carda-Broch

**4:00** —**28.** The effect of imidazolium substituents on the retention properties of surface-confined ionic liquid stationary phases for high performance liquid chromatography. **A. M. Stalcup**, D. S. Van Meter, P. R. Fields, N. Oliver, P. Kodali

**4:25** —**29.** Spectroscopic characterization of proteins in alkylammonium formate ionic liquids for potential application to liquid chromatography. **N. D. Danielson**, W. Wei, S. L. Grossman

### **Astellas USA Foundation Award Lectures in Translational Chemistry: Connecting Basic Research to Improve Human Health**

*Sponsored by PRES, Cosponsored by BIOT, MEDI, ENVR, BIOL, IEC, and HEALTH*

### **Microporous Solid Acid Catalysts**

*Sponsored by CATL, Cosponsored by COLL, FUEL, IEC, and PETR*

### **Presidential Session Celebrating Division Centennials: AGFD, I&EC, ORGN, and PHYS**

*Sponsored by PRES, Cosponsored by AGFD, IEC, ORGN, and PHYS*

## **MONDAY MORNING**

Section A

Radisson Plaza - Warwick -- Chestnut

**Celebrating the 100th Anniversary of the Journal of Industrial and Engineering Chemistry Research**

S. D. Alexandratos, *Organizer*

**9:00 —30.** Advances in molecular modeling of complex fluids: Phase behavior and microstructure in copolymers and associating fluids. **W. G. Chapman**, S. Jain, A. Bymaster, K. R. Cox

**9:30 —31.** Vapor-phase nonideality: The Hayden-O'Connell correlation for 2nd virial coefficients and beyond. **J. P. O'Connell**

**10:00 —32.** Scale-up of a physical vapor deposition evaporation source using thermal and effusion modeling. **B. A. Ogunnaike**, K. Mukati, R. W. Birkmire

**10:30** — Intermission.

**10:45 —33.** A model for cloud points, sorption equilibria, and glass transition temperatures in CO<sub>2</sub> – polymer systems. **A. S. Teja**, A. Kasturirangan

**11:15 —34.** Model predictive controller design for multiple disturbances. M. Kuure-Kinsey, **B. W. Bequette**

**11:45 —35.** Micellization of block copolymers in subcritical and supercritical solvents. **M. Radosz**

Section B

Radisson Plaza - Warwick -- Crystal Ballroom

## **Ionic Liquids: From Knowledge to Application**

### **Interfacial Properties**

J. F. Brennecke, R. D. Rogers, and K. R. Seddon, *Organizers*  
S. Baldelli and A. Podestà, *Organizers, Presiding*

**8:30** — Introductory Remarks.

**8:35 —36.** XPS of ionic liquids: A question of standards? **P. Licence**, R. G. Jones, E. F. Smith, I. J. Villar Garcia

**9:00 —37.** IV-SFG studies on the liquid-liquid interfaces of room temperature ionic liquids ([C<sub>n</sub>mim]PF<sub>6</sub>) contacting molecular liquids. **Y. Ouchi**, D. Kim

**9:25 —38.** Correlation between surface tension and void fraction: Ionic liquids. **C. Larriba**, Y. Yoshida, J. Fernandez de la Mora

**9:50 —39.** Gas-liquid interface analysis of ionic liquids in vacuum. **I. S. Martinez**, S. Baldelli

**10:15** — Intermission.

**10:30 —40.** Interphase formation on reactive metal surfaces in ionic liquids. **P. C. Howlett**, D. R. MacFarlane, M. Forsyth

**10:55 —41.** Elucidating the structure of the room temperature ionic liquid/SiO<sub>2</sub> interface with sum frequency vibrational spectroscopy. J. B. Rollins, **J. C. Conboy**

**11:20 —42.** Influence of solvophobicity and bulk nanostructure on solvation layers of room temperature ionic liquids confined between surfaces. **R. Atkin**, G. G. Warr

**11:45 —43.** Interfacial layering in ionic liquids. **B. M. Ocko**, M. Mezger, H. Reichert, E. Sloutskin, H. Schröder, M. Deutsch, H. Dosch

**12:10 —44.** Investigation of interfacial properties of supported [BMIM][NTf<sub>2</sub>] layers by scanning probe microscopy. **A.**

**Podestà, S. Bovio, P. Milani**

### **Catalytic Synthesis and Utilization of Alcohol**

*Sponsored by CATL, Cosponsored by COLL, FUEL, IEC, and PETR*

### **Fostering Scholarship and Innovation in the Chemical Sciences**

*Sponsored by SOCED, Cosponsored by COMSCI, CHED, and IEC*

## **MONDAY AFTERNOON**

Section A

Radisson Plaza - Warwick -- Chestnut

### **Celebrating the 100th Anniversary of the Journal of Industrial and Engineering Chemistry Research**

S. D. Alexandratos, *Organizer*

**1:30 —45.** Dynamics of flow structures and transport phenomena: Analysis and application. **J. B. Joshi**, M. V. Tabib, S. S. Deshpande, C. S. Mathpati

**2:00 —46.** Phase behavior of supercritical fluid-fluoropolymer mixtures: Application for electrospinning. **M. A. McHugh**

**2:30 —47.** Kinetic modeling of complex processes and catalyst deactivation. **G. F. Froment**

**3:00 —** Intermission.

**3:15 —48.** Effect of H<sub>2</sub>/CO ratio on oxygenate selectivity on promoted Rh catalysts. **J. J. Spivey**, A. Egbebi

**3:45 —49.** Gas-expanded liquids: Versatile media for multiphase catalysis. **B. Subramaniam**

**4:15 —50.** Catalyst development for hydrogen production through reforming of sulfur-containing liquid fuels. S. Lakhaptri, A. Kataria, **M. A. Abraham**

Section B

Radisson Plaza - Warwick -- Crystal Ballroom

### **Ionic Liquids: From Knowledge to Application**

#### **Use In Sensors and Actuators**

J. F. Brennecke, R. D. Rogers, and K. R. Seddon, *Organizers*  
G. A. Baker and X. Zeng, *Organizers, Presiding*

**1:30 —** Introductory Remarks.

**1:35 —51.** Poly(vinyl ferrocene) redox behavior in ionic liquids. Y. Tang, **X. Zeng**

**2:00 —52.** New electrochemical actuators based on polymer gels containing ionic liquids. **M. Watanabe**, Y. Kato, S. Imaizumi, H. Kokubo

**2:25 —53.** Smart systems and materials based on ionic liquids. **T. Erdmenger**, C. Guerrero-Sanchez, R. Hoogenboom, U. S. Schubert

**2:50 —54.** Ionic liquids as electrolytes for electrochemical sensing. **T. J. S. Schubert**, A. Reisinger

**3:15 —** Intermission.

**3:30 —55.** Ionic liquids: Solutions for electrospray ionization mass spectrometry. **J. S. McIndoe**, M. A. Henderson

**3:55 —56.** Biosensors based on ionic liquid platforms. **F. V. Bright**

**4:20 —57.** Inorganic complexes in ionic liquids as oxygen sensors. **J. N. Demas**, S. J. Payne, N. B. Banks, B. B. Hueholt, K. J. Morris, G. A. Baker

**4:45 —58.** Multiplexed hydraulic valve actuation using ionic liquid filled soft channels. **S. Takayama**

### Catalytic Synthesis and Utilization of Alcohol

*Sponsored by CATL, Cosponsored by COLL, FUEL, IEC, and PETR*

## TUESDAY MORNING

Section A

Radisson Plaza - Warwick -- Chestnut

### I&EC Centennial Symposium: 100 Years of Innovation

#### A Century of Innovation Excellence in Industrial and Engineering Chemistry

*Cosponsored by PRES*

W. H. Flank, M. A. Matthews, and M. A. Abraham, *Organizers*

**8:30 —** Introductory Remarks.

**8:40 —59.** Putting science to work: A history of I&EC leadership and innovation in its first hundred years. **W. H. Flank**

**9:10 —60.** Innovation in ammonia synthesis catalysts and technologies. **S. E. Nielsen**

**9:40 —61.** Polyethylene: An account of scientific discovery and industrial innovation. **R. M. Patel**, P. Jain, B. A. Story, S. P. Chum

**10:10 —** Intermission.

**10:30 —62.** The industrial gas industry. **J. Royal**

**11:00 —63.** Membrane separations. **G. Lipscomb**

**11:30 —64.** History of petroleum cracking in the 20th century. **B. H. Davis**, W. H. Flank, A. W. Peters

**12:00 —** Concluding Remarks.

## Section B

Radisson Plaza - Warwick -- Crystal Ballroom

### **Ionic Liquids: From Knowledge to Application**

#### **Material Synthesis in IL's**

J. F. Brennecke, R. D. Rogers, and K. R. Seddon, *Organizers*

J. L. Anthony and A. V. Mudring, *Organizers, Presiding*

**8:30** — Introductory Remarks.

**8:35 —65.** Ionic liquids in China: An overview of recent developments. **U. Welz-Biermann**

**8:55 —66.** Ionic liquids in inorganic synthesis and their influence on the preparation of nanoparticles. **T. J. S. Schubert**, A. Reisinger

**9:15 —67.** Ionic liquids for nanomaterial synthesis. **F. Endres**

**9:35 —68.** Nanoparticles from ionic liquids. **A. V. Mudring**

**9:50 —69.** Preparation of ionic liquids-inorganic nanoparticles hybrid materials: Focus on surface modification of the nanoparticles. **A. Narita**, K. Suzuki, K. Naka, Y. Chujo

**10:05** — Intermission.

**10:25 —70.** Ionic liquids for the synthesis of conducting polymer-noble metal nanocomposites. **J. M. Pringle**, O. Winther-Jensen, C. Lynam, G. G. Wallace, M. Forsyth, D. R. MacFarlane

**10:45 —71.** Ionothermal materials synthesis. **R. E. Morris**

**11:05 —72.** Solubility of silicon dioxide in ionic liquids. X. Sun, **J. L. Anthony**

**11:25 —73.** Colloidal stability of silica particles in ionic liquids and fabrication of ion gels based on colloidal self-assembly. **K. Ueno**, A. Inaba, K. Hata, M. Kondoh, M. Watanabe

**11:40 —74.** Electrodeposition of lithium and lithium-sodium alloys from quaternary ammonium and phosphonium ILs. J. Vega, J. Zhou, **P. A. Kohl**

#### **Catalytic Synthesis and Utilization of Alcohol**

*Sponsored by CATL, Cosponsored by COLL, FUEL, IEC, and PETR*

### **TUESDAY AFTERNOON**

## Section A

Radisson Plaza - Warwick -- Chestnut

### **I&EC Centennial Symposium: 100 Years of Innovation**

#### **The Next Century of Industrial and Engineering Innovation**

*Cosponsored by PRES*

W. H. Flank, M. A. Matthews, and M. A. Abraham, *Organizers*

**1:30** — Introductory Remarks.

**1:40** —**75.** History of fluidized catalytic cracking (FCC): A history of innovation 1942 - 2008. **R. Fletcher**

**2:10** —**76.** Purification of automotive exhaust through catalysis. **M. Rodkin**, S. Tauster, X. Wei, T. Neubauer

**2:40** —**77.** TUD-1: Advanced catalytic materials for the refining and petrochemical industry. **A. Gaffney**

**3:10** — Intermission.

**3:30** —**78.** Evolving production of acetyl chemicals: A mirror for the evolution of the chemical industry. **J. R. Zoeller**

**4:00** —**79.** Ionic liquids: Growth of a field through the eyes of the I&EC division. **R. D. Rogers**

**4:30** —**80.** Vignettes on green chemistry and engineering. **P. G. Jessop**

**5:00** — Concluding Remarks.

Section B

Radisson Plaza - Warwick -- Crystal Ballroom

### **Ionic Liquids: From Knowledge to Application**

#### **Thermophysical Properties**

J. F. Brennecke, R. D. Rogers, and K. R. Seddon, *Organizers*

J. W. Magee and L. P. N. Rebelo, *Organizers, Presiding*

**1:30** —**81.** Vaporization of ionic liquids: A temperature programmed desorption (TPD) study. **P. Licence**, R. G. Jones, K. R. J. Lovelock, A. Deyko, J. A. Corfield

**1:50** —**82.** Characterization of strong and super acids, using protic ionic liquids made with tertiary amine bases: The N-H chemical shift. **J -P. Belieres**, N. Byrne, C. A. Angell

**2:10** —**83.** Development of predictive models for the thermophysical properties of ionic liquids: A first step toward the CAMD of ionic liquids. **J. A. P. Coutinho**, R. Gardas

**2:30** —**84.** Chemical speciation in ionic liquids and their mixtures with polar solvents. **G. Hefter**, R. Buchner, J. Hunger, A. Stoppa

**2:50** — Intermission.

**3:05** —**85.** Temperature and pressure dependencies of isobaric thermal expansivity and isobaric heat capacity of ionic liquids. **J. Troncoso**, P. Navia, Y. A. Sanmamed, D. Gonzalez-Salgado, L. Romani

**3:25** —**86.** Predicting thermophysical properties of ionic liquids. **D. W. Rooney**

**3:45** —**87.** Physicochemical properties and structures of ionic liquids. **H. Tokuda**

**4:05** —**88.** On the nature of ionic liquids. **K. N. Marsh**

### **TUESDAY EVENING**

Pennsylvania Convention Center -- Hall C

### General Posters

M. A. Gonzalez, *Organizer*

#### 8:00 - 10:00

- 89.** Ab initio approaches to understanding polarisability of ionic liquids. **E. I. Izgorodina**, D. R. MacFarlane, M. Forsyth
- 90.** Aldol condensation by hydroxymethanesulfonic acid. **S. Kaur**, S. Sambher, C. Baskar, R. S. Dhillon
- 91.** Application of the CPA EoS to the modeling of biodiesel production. M. B. Oliveira, F. R. Varanda, M. J. Pratas, I. M. Marrucho, A. J. Queimada, **J. A. P. Coutinho**
- 92.** Arsenic and selenium recovery from aqueous systems using nanoporous silica polyamine composites. **V. Kailasam**, E. Rosenberg
- 93.** Chemoselective reduction of aldehyde in the presence of ester by thiourea dioxide. **S. Kaur**, S. Sambher, C. Baskar, R. S. Dhillon
- 94.** Dry-spinning of sol-gel derived mullite fibers. **X. Chen**, L. Gu, G. Sun
- 95.** Electrodeposition of copper on a copper electrode modified by a film of organic adsorbate. B. Demeyev, V. Mogilniy, **M. Nauryzbayev**
- 96.** Extractive deep desulfurization with polymer-based FeCl<sub>3</sub>. **E. Huh**, N. H. Ko, M. Cheong, H. S. Kim
- 97.** In situ time-resolved characterization of manganese oxide octahedral molecular sieves catalysts during the water-gas shift reaction. **S. Sithambaram**, W. Wen, J. C. Hanson, S. L. Suib
- 98.** Investigation of gas production behavior from organic wastes in a down-draft gasifier. **T. Min**, J. Yun, S. Keel, S. Roh, W. Kim
- 99.** Low NO<sub>x</sub> application of SNCR and two staged reaction for a FRP direct melting process. J. Yun, S. Keel, W. Kim, **T. Min**, S. Roh
- 100.** Oil and water repellency low temperature plasma treated nylon and polyester fibers. **C -W. Kan**, C. W. M. Yuen, S. Q. Jiang, Y. L. Lam
- 101.** Properties monitoring of produced polyacrylamide from three polymer flooding reservoirs. **Y. Wang Sr.**, J. Zhang Sr., W. Zhao Sr.
- 102.** Pyrolysis and gasification-melting characteristics of automobile shredder residue. W. Kim, S. Roh, **T. Min**, J. Yun, S. Keel
- 103.** Selective 1, 4-reduction of unsaturated carbonyl compounds with Thiourea dioxide. **S. Kaur**, S. Sambher, C. Baskar, R. S. Dhillon
- 104.** Selective removal of sulfones in diesel for the low sulfur diesel production. **C. H. Ko**, H -J. Jeon, K. B. Yi, J -H. Park, H. Ahn, G. T. Kim, J -N. Kim
- 105.** Structural design at the polymer-surface interface in nanoporous silica polyamine composites. **V. Kailasam**, E. Rosenberg, J. J. Allen, J. L. Wood, M. A. Hughes
- 106.** Synthesis of 1-(3-phenylpropyl)-pyrrolidine-2,5-dione under solid-liquid phase-transfer catalytic reaction. **M -L. Wang**, C -J. Chen

- 107.** Synthesis of hydrofluoroethers for the development of alternatives of chlorofluorocarbon. **J. E. Kang**, J. Palgunadi, J. S. Lee, M. Cheong, H. S. Kim
- 108.** Synthesis of spherical poly (glycidyl methacrylate) (PGMA) particles in compressed liquid dimethyl ether. **K. S. Oh**, D. W. Cho, W. Bae, Y. W. Lee, H. Kim
- 109.** Technology of processing carbon containing materials of Kazakhstan and their role in production. S. Yefremov, S. Nechipurenko, V. Mogilniy, **M. Nauryzbayev**
- 110.** Wettability and dryability of low temperature plasma treated nylon and polyester fibers. **C -W. Kan**, C. W. M. Yuen, S. Q. Jiang, Y. L. Lam

Section B

Pennsylvania Convention Center -- Hall C

**Ionic Liquids: From Knowledge to Application**

J. F. Brennecke and K. R. Seddon, *Organizers*  
 R. D. Rogers, *Organizer, Presiding*

**8:00 - 10:00**

- 111.** Caffeine ionic liquids – dream or reality? **G. Gurau**, K. Rogers, R. D. Rogers
- 112.** Liquid ion pairs and dimeric anions: Variations on pharmaceutical ionic liquids. **D. R. MacFarlane**, J. L. Scott, K. Fraser, M. Forsyth, E. I. Izgorodina, K. Johansson
- 113.** Pyridine and nicotine as solvents for ionic liquids with related cationic structure. Z. P. Visak, A. Rodriguez, A. B. Pereiro, **J. N. A. Canongia Lopes**, **L. P. N. Rebelo**
- 114.** Comparative toxicity of branched and straight chain alkyl functionality in ionic liquids. **C. McEntee**, J. Gwon, X. Li, J. F. Wishart, S. I. Lall-Ramnarine
- 115.** Degradability by design: 1-Hydroxyimidazole-derived salts as stable, yet degradable ionic liquids. G. Laus, **A. Schwaerzler**, M. Hummel, K. Wurst, V. Kahlenberg, G. Bonn, H. Schottenberger
- 116.** Designed to decompose: Task-specific ionic liquids incorporating N-acylium and N-sulfonylium cations. **K. Gaines**, J. H. Davis Jr., R. A. O'Brien, K. M. Mattson
- 117.** Task-specific ionic liquids (TSILs) based on heterocyclic cations with directly ring-attached aldehyde and benzoyl groups: Hydrate and acetal formation. **K. M. Mattson**, J. H. Davis Jr., R. A. O'Brien, K. Gaines
- 118.** New Bronsted acidic TSILs. From computation-guided design to synthesis and properties. **J. H. Davis Jr.**, R. A. O'Brien, K. M. Mattson, K. Gaines, B. B. Plash, A. Wierzbicki, E. A. Salter
- 119.** New amine functionalized ionic liquids for multimode acid gas capture. **J. H. Davis Jr.**, R. A. O'Brien, K. Gaines, K. M. Mattson
- 120.** Study of ionic liquid solvation and aggregation by NMR spectroscopy and molecular dynamics simulations. **R. C. Remsing**, Z. Liu, B. B. O'Brien, G. Moyna
- 121.** Specific interactions between salts and ionic liquids in aqueous salt solutions. L. I. N. Tomé, F. R. Varanda, M. G. Freire, I. M. Marrucho, **J. A. P. Coutinho**
- 122.** Solvation of a small peptide molecule in room-temperature ionic liquids. **Y. Shim**, H. J. Kim
- 123.** Synthesis and properties of ionic liquids derived from N-methyl-D-glucamine. **G. Chalumot**, J. L. Anderson

124. Decomposition of the ionic liquid 1-ethyl-3-methylimidazolium ethylsulfate under ambient conditions. **L. E. Ficke**, J. F. Brennecke
125. Novel luminescent and magnetic ionic crystals. **A. V. Mudring**
126. Template-free recyclable growth of magnetite nanocrystals in neat ionic liquid. **J. D. Woodward**, A. J. Rondinone, G. A. Baker
127. Molar refraction in a series of imidazolium- and phosphonium-based ionic liquids. M. Tariq, **J. N. A. Canongia Lopes**, **L. P. Rebelo**
128. Phase equilibria in ionic liquid plus aromatic compound binary systems. M. Blesic, **J. N. A. Canongia Lopes**, **L. P. Rebelo**
129. Self-aggregation and fluorescence quenching of surfactant ionic liquids. M. Blesic, A. Lopes, E. Melo, Z. Petrovski, N. Plechkova, J. N. A. Canongia Lopes, K. R. Seddon, **L. P. Rebelo**
130. Tetraalkylphosphonium polyoxometalates as novel ionic liquids. **M. L. Dietz**, P. G. Rickert, M. R. Antonio, M. A. Firestone, J. F. Wishart, T. Szreder, K. -A. Kubatko
131. Improved chemical analysis of lignocellulosic biomass through dissolution into ionic liquids. L. M. Kline, R. Jena Kumar, **D. G. Hayes**, N. Labbe
132. Utilizing elongational flow in the spinning of carbon fiber precursors from 1-butyl-3-methylimidazolium chloride cellulose solutions. **R. Sammons**, J. Collier, T. Rials, S. Petrovan
133. Shear rheology of 1-butyl-3-methylimidazolium chloride cellulose solutions including solution character and preparation. **J. R. Collier**, **J. Watson**, B. Collier, S. Petrovan
134. Molecular dynamics simulations of cellobiose in the ionic liquid 1-n-butyl-3-methylimidazolium chloride. **Z. Liu**, R. C. Remsing, P. B. Moore, G. Moyna
135. Development of the polymer actuator based on the polymer electrolyte composed of ionic liquids and ABA-type triblock copolymers. **S. Imaizumi**, Y. Kato, H. Kokubo, M. Watanabe
136. Development of ionic liquid/polyimide copolymers for CO<sub>2</sub>/H<sub>2</sub> membranes. **P. Li**, Q. Zhao, J. L. Anderson, M. R. Coleman
137. Thermodynamics properties for imidazolium ionic liquids + methyl methacrylate. **W. Fan**, Q. Zhou, R. Yan, **S. Zhang**
138. Imidazolium-based zwitterionic compounds bearing a fluorinated alkyl group and a sulfonate group for proton exchange membrane. **H. Kim**, J. S. Lee, M. Cheong, H. S. Kim
139. Generation and detection of radicals in ionic liquids. **J. A. C. Clyburne**, K. Ghandi, C. Walsby
140. Hydrogen halide-equivalent ionic liquids: Application in the ring opening of epoxides. **J. Salazar**, J. M. Rodriguez, S. E. Lopez
141. Kinetic study of S-alkylation of 2-mercaptobenzimidazole by allyl bromide in the presence of potassium hydroxide. **M - L. Wang**, Y -C. Liu
142. Electrochemical studies of the Fries rearrangement in ionic liquids. **G. T. Cheek**
143. Kinetic studies of rapid alkylation reaction in liquid-liquid biphasic reaction using acidic ionic liquid catalyst. **J. Joni**, P. Wasserscheid
144. Liquid-liquid electrochemistry of a new class of chiral hydrophobic room temperature ionic liquids. **J. B. Rollins**, J. C. Conboy
145. Atomistic modeling of densities and solubility parameters of ionic liquids. **B. Derecskei**, A. Derecskei-Kovacs

- 146.** Atomistic simulation of the thermodynamic properties of organic hydrazine-derivatives and hydrazinium-based energetic salts and ionic liquids. **K. E. Gutowski**, B. Gurkan, S. Jayaraman, E. J. Maginn
- 147.** Considering partial ionic dissociation with electrolytic excess Gibbs energy models in an asymmetric framework. **L. D. Simoni**, A. A. Augugliaro, J. F. Brennecke, M. A. Stadtherr
- 148.** The potential energy landscape of bis(fluorosulfonyl)amide. K. Shimizu, Y. Umabayashi, K. Fujii, **A. A. H. Pádua**, **J. N. A. Canongia Lopes**
- 149.** Vibrational spectrum of [emin][TF2N] ion pair: A density functional study. **N. R. Dhumal**, H. J. Kim
- 150.** Solubility of gases in [hmim][Tf2N] and [hmim][eFAP]. **Z. K. Lopez-castillo**, D. E. Kestel, J. F. Brennecke
- 151.** Gas sorption properties of ionic liquids. **Q. Zhao**, P. Li, M. R. Coleman, J. L. Anderson
- 152.** High-pressure solubilities of carbon dioxide in [Cnmim][Tf2N] ionic liquids. P. J. Carvalho, J. J. B. Machado, J. Pauly, J.-L. Daridon, I. M. Marrucho, **J. A. P. Coutinho**
- 153.** Readily prepared and cost effective ionic liquids: Few steps more toward the industrial application of CO<sub>2</sub> separation using ionic liquids. H. S. Kim, **J. Palgunadi**, J. E. Kang
- 154.** Light gas separation with gelled room-temperature ionic liquid supported membranes. **B. A. Voss**, J. E. Bara, D. L. Gin, R. D. Noble
- 155.** Pure gas solubilities and viscosities of task-specific ionic liquids. **D. E. Kestel**, D. F. Rahill, J. C. de la Fuente, J. F. Brennecke
- 156.** Separation of liquids with triethylsulphonium bis(trifluoromethylsulfonyl)-imide ionic liquid. **A. Marciniak**, U. Domańska-Żelazna
- 157.** ILTHERMO: Archival storage and retrieval of thermophysical properties. **J. W. Magee**, Q. Dong, C. D. Muzny, A. Kazakov, V. Diky, J. A. Widegren, R. D. Chirico, K. N. Marsh, M. Frenkel
- 158.** Solubility of fluorinated compounds in ionic liquids. R. Ferreira, M. Blesic, J. Trindade, I. M. Marrucho, **J. N. A. Canongia Lopes**, **L. P. Rebelo**
- 159.** Influence of the anionic species of a molten salt on lipid organization. **K. O. Evans**
- 160.** Interfacial mass transport in biphasic ionic liquid/organic solvent systems. A. Ahosseini, L. Weatherley, **A. M. Scurto**
- 161.** LCST behavior of linear polymers and polymer gels in ionic liquids and its possibility in material science. **M. Watanabe**, T. Ueki, K. Kodama, A. Yamaguchi
- 162.** Transport properties of ionic liquids. **S. S. Moganty**, R. E. Baltus, P. Goonetillake, D. Roy

## WEDNESDAY MORNING

Section A

Radisson Plaza - Warwick -- Chestnut

### Ionic Liquids: From Knowledge to Application

#### Molecular Simulations

J. F. Brennecke, R. D. Rogers, and K. R. Seddon, *Organizers*  
P. Ballone and E. J. Maginn, *Organizers, Presiding*

**8:30** — Introductory Remarks.

**8:35** —**163.** Interactions, structure and properties of ionic liquids from molecular simulation. **A. A. H. Pádua**, J. N. A. Canongia Lopes, M. F. Costa Gomes, A. Sanmartín Pensado

**9:00** —**164.** Theoretical predictions of the structure and properties of ionic liquids. **M. S. Gordon**, J. A. Boatz

**9:25** —**165.** First-principles evaluation of CO<sub>2</sub> complexation in functionalized ionic liquids. **W. F. Schneider**, E. Mindrup

**9:50** —**166.** Dynamics and spectroscopy in room temperature ionic liquids. **C. J. Margulis**

**10:15** — Intermission.

**10:35** —**167.** Solvation, dielectric relaxation and ion conductivity in the mixture of 1-butyl-3-methylimidazolium hexafluorophosphate and supercritical carbon dioxide. Y. Shim, **H. J. Kim**

**11:00** —**168.** Ionic to dipolar transition in [bmim][PF<sub>6</sub>] / naphthalene mixtures: A computational study. **M. G. Del Popolo**

**11:25** —**169.** Multiscale simulation of ionic liquids for process innovation. **S. Zhang**, X. Liu, L. Yu

Section B

Radisson Plaza - Warwick -- Crystal Ballroom

### **Environmental and Economic Metrics for Green Technologies**

*Cosponsored by Green Chemistry and Engineering Sub-Division*  
M. A. Gonzalez and P. G. Jessop, *Organizers*

**9:00** —**170.** Conversion of ethylene in dry gas via oligomerization over solid catalysts. **D. Xue**, L. Chunyi, Y. Chaohe, S. Honghong

**9:25** —**171.** Copper nanoparticles recycled from copper chloride containing waste etchants using microemulsion method. **K - S. Lin**, Z -P. Wang, K -Y. Li

**9:50** —**172.** Process and 2-D nucleation mechanism of high-bond-strength replacement copper plating on iron. **L. Feng**, **F. Hu**, **S. Feng Sr.**

**10:15** —**173.** Proline catalyzed aldol reactions in supercritical fluids. L. Liu, Z -W. Liu, **Z -T. Liu**

**10:40** —**174.** Study of gis-based vehicle emission inventory in Hangzhou urban-area. **Y. Wei**, **Q. Zhang**, **W. Tian**

**11:05** —**175.** Study on performance of EMD mixed with rare-earth metal oxide. **L. Feng**, **F. Hu**, **S. Feng Sr.**

**11:30** —**176.** Synthesis and fine structure characterization of anatase titania nanotubes for basic dye wastewater treatment. **K -S. Lin**, C -S. Chang, K -Y. Li

**11:55** —**177.** Vehicle emission prediction in different energy scenarios from 2005 to 2030. J. Xu, **W. Tian**, **Q. Zhang**, **Y. Wei**

### **Catalyst and Process for Biorenewable Energy**

*Sponsored by CATL, Cosponsored by COLL, FUEL, IEC, and PETR*

### **WEDNESDAY AFTERNOON**

## Section A

Radisson Plaza - Warwick -- Chestnut

### **Ionic Liquids: From Knowledge to Application**

#### **Pharmaceutical Applications**

J. F. Brennecke and K. R. Seddon, *Organizers*  
D. R. MacFarlane and R. D. Rogers, *Organizers, Presiding*

**1:30** — Introductory Remarks.

**1:35 —178.** An anticrystal engineering approach to functional ionic liquids. **J. L. Scott**, D. R. MacFarlane, P. Dean, J. Turanjanin, R. D. Rogers

**2:00 —179.** Ionic liquids: Media for studying the protein folding problem. **C. A. Angell**, N. Byrne

**2:25 —180.** The development of ionic liquids for biomedical applications. **G. D. Elliott**, R. Kemp, D. R. MacFarlane, K. Fujita, M. Forsyth

**2:50 —181.** Protein denaturation by ionic liquids and the Hofmeister series. **H. Weingärtner**, D. Constantinescu, C. Herrmann

**3:15** — Intermission.

**3:35 —182.** Ionic liquids as solvents for the synthesis of active pharmaceutical ingredients. **T. Beyersdorff**, T. J. S. Schubert

**4:00 —183.** Sweetener and antibacterial ionic liquids. **W. L. Hough-Troutman**, M. Smiglak, J. Pernak, D. T. Daly, R. D. Rogers

**4:25 —184.** Frozen ionic liquids: A new breed of nanomaterials. **B. El-Zahab**, A. Tesfai, D. K. Bwambok, G. A. Baker, M. Lowry, S. O. Fakayode, I. Warner

**4:50 —185.** Ionic liquids: Opportunities and challenges in biopharmaceutical stabilization. **J. Hey**, T. Martinelli, D. Maher

### **THURSDAY MORNING**

## Section A

Radisson Plaza - Warwick -- Chestnut

### **Ionic Liquids: From Knowledge to Application**

#### **Industrial Applications**

J. F. Brennecke, R. D. Rogers, and K. R. Seddon, *Organizers*  
P. F. H. Schwab and M. B. Turner, *Organizers, Presiding*

**8:30** — Introductory Remarks.

**8:35 —186.** Liquid-liquid-biphasic hydrosilylation in a continuous loop reactor: From ionic liquid selection to miniplant design and operation. **P. Wasserscheid**, N. Hofmann, P. S. Schulz, T. Frey, V. Stanjek

**9:05 —187.** The commercialization of ionic liquids: The view of an established start-up company. **T. J. S. Schubert**, A. Reisinger

**9:20 —188.** New trends in the industrial production and quality management of ionic liquids. **T. J. S. Schubert**, T. Beyersdorff, M. H. Klingele

**9:35 —189.** Industrial application of ionic liquids: Challenges and opportunities. **P. F. H. Schwab**, M. Seiler

**10:05 —** Intermission.

**10:20 —190.** Converting properties into products: The development of high performance lubricants and antistatic additives. **M. Wagner**, M. Uerdingen

**10:50 —191.** Ionic liquids as green solvents: An ecological assessment. **D. Reinhardt**, D. Kralisch, F. Ilgen, G. Kreisel, B. Koenig

**11:20 —192.** Solubility of fluorinated compounds in room-temperature ionic liquids. **M. B. Shiflett**, A. Yokozeki

## THURSDAY AFTERNOON

Section A

Radisson Plaza - Warwick -- Chestnut

### Ionic Liquids: From Knowledge to Application

#### General Session

J. F. Brennecke, R. D. Rogers, and K. R. Seddon, *Organizers*

J. H. Davis Jr. and P. Wasserscheid, *Organizers, Presiding*

**1:30 —193.** Highly efficient and selective C-H-activation in gallium containing molten salt systems: Toward a fundamentally new route for CH<sub>4</sub> valorization. **P. Wasserscheid**, T. Weiss, F. Agel

**1:50 —194.** Labile bonds and ionic liquids: An emerging paradigm relating utility to fragility. **J. H. Davis Jr.**

**2:10 —195.** Ionic liquid complexes for biphasic catalysis: An “extract” science. **R. D. Singer**, P. U. Naik

**2:30 —196.** Use of multinuclear NMR spectroscopy and molecular dynamics simulations in the study of ionic liquid structure, solvation, and dynamics. R. C. Remsing, Z. Liu, J. L. Wildin, A. L. Rapp, I. D. Petrik, B. B. O'Brien, B. L. Walter, **G. Moyna**

**2:50 —197.** Carbonylation of methanol and olefins without the use of alkyl halide. **A. J. Vetter**, J. R. Zoeller, M. K. Moore, T. Barnette, A. Quillen

**3:10 —198.** Ionic liquids in tribology. **B. J. Kinzig**, M. J. Purdon, G. Claycomb, P. Sutor Sr.

**3:30 —199.** Application of ionic liquids for fuel cells. **V. Hacker**, E. Wallnoefer, B. Wieser, R. Kalb

**3:50 —200.** Protocols for halide free synthesis of ionic liquids via hydrogen carbonate precursors. **M. Smiglak**, R. D. Rogers

**4:10 —201.** Ionic liquid radiation chemistry and its implications for their use in nuclear fuel processing. **J. F. Wishart**

**4:30 —202.** Main-chain ionic polymers: The next generation of ionic liquid-inspired polymer platforms. **T. K. Carlisle**, J. E. Bara, C. J. Gabriel, R. D. Noble, D. L. Gin

**4:50 —203.** Thermomorphic organic liquid-ionic liquid systems: Characterization of phase separation by conductivity and spectroscopy. **A. Riisager**, R. W. Berg, P. Wasserscheid, R. Fehrmann

**5:10 —204.** Organic electrochemistry in ionic liquids. **S. T. Handy**