

Monday, March 18, 2024 | 2pm – 6pm session

Ernest N. Morial Convention Center | Hall B, Rm. 4

Separation and Reactivity in and of Ionic Liquids | S. Garrett-Roe, *Presiding*

2:00 PM. Materials design of amino acid ionic liquids for CO₂ capture and conversion: a multiscale theory/modeling. **B. Yoon**, G.A. Voth

2:15 PM. Efficient implementation of the test particle insertion method for high-throughput screening of gas absorption in ionic liquids. R. Smith, **E. Maginn**

2:30 PM. Tailoring ionic liquids for gas separation. **S. Dai**

3:00 PM. Modulating chemical and physical sorption of CO₂ and SO₂ in carboxylate ionic liquids to improve capture and selectivity. **A. Padua**, N. Scaglione, J. Avila, E. Bakis, M. Costa Gomes

3:30 PM. Intermission

3:45 PM. Time-resolved nonlinear spectroscopy of excess electrons in aliphatic ionic liquids. A.T. Healy, C. Huber, M. Knudtzon, **D.A. Blank**

4:15 PM. Effect of solvation heterogeneity in ionic liquids on fundamental chemical reaction dynamics analyzed by time-resolved spectroscopy. **Y. Kimura**, K. Fujii

4:45 PM. CO₂ chemisorption behavior in conjugated carbanion-derived ionic liquids via carboxylic acid formation. **Z. Yang**, S.M. Mahurin, L. Qiu, N. Mokhtarinori, S. Dai

5:00 PM. Digital engineering of ionic liquid rocket propellants: A machine learning approach. **G.L. Vaghjiani**

5:15 PM. Unsupervised reaction pathways search for the oxidation of hypergolic ionic liquids. K. Fujioka, R. Kaiser, **R. Sun**

5:45 PM. Unraveling the hypergolicity and reactivity of ionic liquids exploiting the chirped-pulse droplet merging manipulation in an ultrasonic levitator. **S. Biswas**, K. Fujioka, I. Antonov, G. Rizzo, D. Paul, S. Chambreau, S. Schneider, R. Sun, R. Kaiser

Tuesday, March 19, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | Hall B, Rm. 4

Structure and Dynamics | K. Shimizu, *Presiding*

8:15 AM. Trends in ionic liquid diffusion in graphite slit pores from molecular dynamics simulation and machine learning. **J.A. Greathouse**, D. Poe, S. Bobbitt, J. Keth, J. Allers, J. Harvey, T.M. Alam

8:30 AM. Structure for the sake of structure or the structural origin of structural dynamics? (AKA how do we understand viscosity in ILs?). **C.J. Margulis**

8:45 AM. Intermission.

9:15 AM. Strengths, distributions and life times of hydrogen bonds in hydroxyl-functionalized ionic liquids. **R. Ludwig**, J. Neumann, D. Paschek, D. Kolokolov

9:45 AM. Effects of electric charge, dipole moment, and molecular size on the viscosity of ionic liquids. J. Itliong, A.L. Frischknecht, M.J. Stevens, **I. Nakamura**

10:00 AM. Intermission.

10:15 AM. Cyanoborates: Low-viscosity ionic liquids for electrochemical applications. **M. Finze**

10:45 AM. Unraveling stability and flow dynamics: Porous suspensions of metal-organic frameworks in ionic liquids. **M. Costa Gomes**, C. Correa, G. Legrand, T. Divoux, S. Manneville, A. Padua

11:15 AM. Chirality transfer and Grotthuss diffusion in ionic liquids. **B. Kirchner**

11:45 AM. Electric field gradient fluctuations around sodium cations in ionic liquids. **C. Rumble**, K. Dziubinska-Kühn

Tuesday, March 19, 2024 | 2pm – 6pm session

Ernest N. Morial Convention Center | R05

Structure and Dynamics | S. Roy, *Presiding*

2:00 PM. Investigating local interactions between ions of like charge in carboxyl-functionalized ionic liquids.

P.A. Harville, O. Moss, A. Rana, E. Bocanegra, M.A. Johnson

2:15 PM. Filling the gaps in our understanding of ionic liquids: The study of homobaric ionic liquids. **T. Welton**,

S. Koutsoukos

2:45 PM. Exploring structural heterogeneities in ionic liquids: Insights from molecular dynamics simulations.

A.A. Freitas, J. Canongia Lopes, **K. Shimizu**

3:15 PM. Describing ionic liquid systems: Partial charges, charge transfer and polarizability. **P. Hunt**

3:45 PM. Intermission.

4:00 PM. Structural and dynamical features of molten salts: From speciation to network formation. **S. Roy**,

A. Ivanov, V. Bryantsev, M.S. Emerson, F. Wu, S. Sharma, C.J. Margulis, H. Wang, E. Maginn, Y. Liu, S. Gill, A. Frenkel, J.F. Wishart

4:30 PM. Solving molten salt structure puzzles with Raman spectroscopy and simulations. **V. Bryantsev**,

S. Roy, L. Gibson

5:00 PM. Solid state of ionic liquids: How crystallography helps rationalize the properties of ionic liquids.

P. Hillesheim, A. Mirjafari, M. Zeller, G. Guillet

5:15 PM. Solvent structure effects on the physicochemical properties, ionic association, and complex cation stability of solvate ionic liquids. **C.M. Burba**

5:30 PM. Quantum chemistry-driven machine learning approach for the prediction of physical properties of ionic liquids. **M. Mood**, M.K. Kidder, B.A. Simmons, J. Smith

5:45 PM. Investigating the effect of branching on physical properties for alkyl phosphonium-based ionic liquids.

R. Blanski, M. Perone, N. Redeker, K.B. Ghiassi

Wednesday, March 20, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | R09

Interfaces and Electrochemical Applications | J. Pringle, *Presiding*

8:15 AM. Pyrlium- and pyridinium-based ionic liquids as friction modifiers for naphthenic greases.

M. Chacon Teran, C. Moustafa, J. Luu, A. Martini, M. Findlater

8:30 AM. Buoy effect - surface enrichment of Pt complexes in ionic liquid solutions by ligand design.

H.-P. Steinrueck

9:00 AM. IV-SFG studies on electric double layer structure at ionic liquid/aqueous electrolyte solution interfaces. **Y. Ouchi**

9:15 AM. Electrical double layer of salt-in-ionic liquids. **R.M. Espinosa-Marzal**, X. Zhang, Z.A. Goodwin, A. Hoane, A. Deptula, H. Li, Q. Zheng, M. Rutland, R. Atkin, A. Gewirth

9:30 AM. Intermission.

9:45 AM. Lithium deposition and solid-electrolyte interphase formation in bis(fluorosulfonyl)amide ionic liquids.

Y. Katayama, S. Kato, R. Yamashita, N. Serizawa

10:15 AM. Superior electrically conductive deep eutectic solvents using iodine. **H. Shirota**

10:45 AM. Development of ionic electrolytes by tailoring the ionic and molecular structure. **J. Pringle**,

F. Vallana, F. Makhlooghiazad, A. Sourjah, A. Warrington, M. Forsyth

11:15 AM. Structure and dynamics of water-in-salt LiTFSI electrolytes from first-principles molecular dynamics simulation. **J.I. Siepmann**, R. Singh, X. Lin, Y. Zhang, E. Maginn, P.T. Cummings

Wednesday, March 20, 2024 | 2pm – 6pm session

Ernest N. Morial Convention Center | R07

Structure and Dynamics and Boronium Ionic Liquids | J. Wishart, S. Shaw, *Presiding*

2:00 PM. Phase transitions in ionic liquids. **S.K. Shaw**

2:15 PM. Experimental evidence of liquid-liquid transition in ionic liquids. **J. Sangoro**

2:45 PM. Understanding the rotational dynamics and interactions in 1-ethyl-3-methylimidazolium methylphosphonate and its mixtures with methyl imidazole: Pulsed NMR and bulk property measurements and DFT calculations. S. Sagala, J. Kaur, C. Hicks, **E.L. Quitevis**

3:15 PM. Ultrafast vibrational spectroscopy of ionic liquids for proton transport and CO₂ capture. **S. Garrett-Roe**

3:45 PM. Atomic resolution measurements of structure and dynamics in ionic liquids using magic-angle-spinning NMR. G.R. Acharya, D. Grajeda, **A.J. Nieuwkoop**

4:15 PM. Intermission.

4:30 PM. Development and characterization of novel boronium ionic liquid electrolytes. **C.D. Stachurski**, J.H. Davis, N.E. Larm, T. Cosby, P.C. Trulove, D.P. Durkin

4:45 PM. Expanding the scope of boronium cations potentially suitable for use in creating ionic liquids. **J.H. Davis**, M.E. Crowley, C.D. Stachurski, M. Zeller, N.E. Larm, D.P. Durkin, P.C. Trulove

5:15 PM. Considering Neoteric boronium ionic liquids for supercapacitor applications. **D.P. Durkin**, C.D. Stachurski, T. Cosby, C.M. Kinnaman, N.E. Larm, J.H. Davis, P.C. Trulove

5:45 PM. Radiation chemistry of boronium ionic liquids. **J.F. Wishart**, F. Wang, J.H. Davis, M.E. Crowley, M.G. Ballentine

Thursday, March 21, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | R07

Mixtures, Deep Eutectics and Applications | J. G. McDaniel, *Presiding*

8:00 AM. Lipid-Like ionic liquids for cocrystallization of long-chain alkyl halides: From serendipity to rational design. M. Musozoda, P. Hillesheim, **A. Mirjafari**

8:15 AM. Designing the designer solvent: Investigating the structural phase behavior of binary imidazolium-based ionic liquid molecular cosolvent mixtures. **C.B. Lasar**, M.L. Cousineau, K.J. Gundenkauf, D. Duffy, B.J. Bellott, S.K. Shaw

8:30 AM. Miscibility and phase behavior of ionic liquid/water mixtures. **J.G. McDaniel**

9:00 AM. Ionic liquids and their mixtures for lubrication and supercapacitors: Bulk and interfacial self-assembly, interphase transitions and electroresponsivity. **M.W. Rutland**

9:30 AM. Not confused protons, just shared: A study of the pseudo-protic ionic liquid formed by mixtures of 1-methylimidazole and acetic acid. L. Wang, **D.G. Kuroda**

9:45 AM. Diphenylalanine self-assembly in aqueous ionic liquids: Mixed United-atom/coarse-grained model with adaptive parameterization. **J. Ma**

10:00 AM. Intermission.

10:15 AM. Decoupling between the charge transport and structural dynamics in ionic liquids, polymerized ionic liquids and ionic nanocomposites. **Z. Wojnarowska**, M. Paluch

10:45 AM. Are zwitterionic liquids special? **G.A. Baker**, P. Ishtaweera

11:15 AM. Probing ionic systems within aerosols, deep eutectic solvents, & plastic crystals with X-Ray and Raman Spectroscopy. **M. Ahmed**, P. Kim, C. Weeraratna, N. Dias, A. Lemmens, S. Nemsak, K.R. Wilson

11:30 AM. Exploiting chirality in ionic liquids and deep eutectic solvents to induce circularly polarized luminescence. **T. Hopkins**