Curriculum Vitae
Edward J. Maginn

Work Address

Department of Chemical and Biomolecular Engineering
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Higher Education

Ph.D. Chemical Engineering, University of California, Berkeley, CA (1995).
B.S. Chemical Engineering, Iowa State University, Ames IA (1987).

Professional Experience

2013	Dorini Family Chair of Energy Studies, University of Notre Dame
2012-present	Chair, Department of Chemical and Biomolecular Engineering, University of Notre Dame
2009-2012	Associate Dean for Academic Programs, The Graduate School, University of Notre Dame
Fall 2007	Visiting Scientist, Computer Science Research Institute, Sandia National Laboratories, Albuquerque, NM
2005-present	Professor, Department of Chemical Engineering University of Notre Dame, Notre Dame, IN
2000-2005	Associate Professor, Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN
1995-2000	Assistant Professor, Department of Chemical Engineering University of Notre Dame, Notre Dame, IN
1987-1990	Process Engineer, Procter and Gamble Company, Iowa City, IA

Distinctions, Honors, Awards, Fellowships

- James A. Burns C.S.C. Award for Distinction in Graduate Education, Notre Dame Graduate School, 2018.
- Founding Series Editor, *Molecular Modeling and Simulation: Applications and Perspectives*, Springer Nature, 2015-present
- Fellow, American Association for the Advancement of Science, 2010.
- Inaugural Early Career Award, Computational Molecular Science and Engineering Forum of the American Institute of Chemical Engineers, 2009.
- Trustee, Computer Aids for Chemical Engineering (CAChE) Corporation, 2009-present.
- BP Notre Dame College of Engineering Outstanding Teacher Award, 2006.
- John A. Kaneb Award for outstanding teaching, University of Notre Dame, 2001, 2006.
- AIChE Student Chapter Outstanding Teaching Award, Notre Dame Chemical Engineering (1998, 2000).

- ASEE Dow Outstanding New Faculty Award (1998).
- NSF Faculty Early Career Development (CAREER) Award (1997).
- Teaching Effectiveness Award, University of California Graduate Division (1994).
- Outstanding Graduate Student Instructor - Berkeley Chemical Engineering (1993 and 1994).
- Cardinal Key, Iowa State University's highest honor society (1987).

Professional Memberships

- American Institute of Chemical Engineers, American Chemical Society, Tau Beta Pi, International Zeolite Association, American Association for the Advancement of Science.

Patents

J. F. Brennecke and E. J. Maginn, "Purification of Gas With Liquid Ionic Compounds", US Patent 6,579,343, issued 6/17/03.

A. E. Ostafin, R. Nooney and E. J. Maginn, "Process for Making Mesoporous Silicate Nanoparticle Coatings and Hollow Mesoporous Silica Nano-Shells", US Patent 6,913,825, issued 7/5/2005.

M. Muldoon, J. F. Brennecke, E. J. Maginn, E. F. Scriven, C. H. Mcateer and R. Murugan, "Aminopyridinium Ionic Liquids", US Patent 7,687,513, issued March 30, 2010.

W. F. Schneider, J. F. Brennecke, E. J. Maginn, E. Mindrup, B. Gurkan, E. Price and B. Goodrich. "Ionic Liquids Comprising Heteraromatic Anions", US Patent 9,951,008, issued April 24, 2018.

Patrick Benaben, Joan Brennecke, Edward Maginn and Mauricio Quiroz-Guzman, "Ionic Liquid Electrolyte and Method to Electrodeposit Metals", PCT/US2015/025706; WO2015160776A1, April 4, 2015.

Saeed Moghaddam, Abhilash Paneri and Edward J. Maginn, "Ionic Liquid-Based Absorption Cooling System with High Coefficient of Performance", PCT/US2016/053881; WO2017/058747, March 22, 2018.

Books, Monographs, Book Chapters

1. A. T. Bell, E. J. Maginn and D. N. Theodorou, "Molecular Simulation of Adsorption and Diffusion in Zeolites", in *Handbook of Heterogeneous Catalysis,* G. Ertl, H. Knozinger, and J. Weitkamp, (eds), VCH, Weinham, **1997**.
2. Joan F. Brennecke and Edward J. Maginn, "Gas Solubilities in Ionic Liquids," in *Ionic Liquids in Synthesis*, P. Wasserscheid and T. Welton, Eds., Wiley-VCH, **2003**, p. 81-93.
3. Jessica L. Anderson, Jennifer L. Anthony, Joan F. Brennecke and Edward J. Maginn, "Gas Solubilities in Ionic Liquids", in *Ionic Liquids in Synthesis*, 2nd edition, P. Wasserscheid and T. Welton, Eds., Wiley, **2007**.
4. Patricia Hunt, Edward J. Maginn, Ruth M. Lynden-Bell and Mario G. Del Popolo, "Computational Modelling of Ionic Liquids", in *Ionic Liquids in Synthesis*, 2nd edition, P. Wasserscheid and T. Welton, Eds., Wiley, **2007**.
5. Edward J. Maginn, "Atomistic Simulation of Ionic Liquids" in *Reviews in Computational*

Chemistry, Kenny B. Lipkowitz, and Tom Cundari, (Eds)., Wiley, Hoboken, NJ, **2009**.

6. Jindal K. Shah and Edward J. Maginn, "Molecular Simulation of Ionic Liquids: Where We Are and the Path Forward" in *Ionic Liquids COILed for Action*, Ken Seddon, Robin Rogers and Natalia Plechkova (eds), Wiley, **2013**.
7. "Foundations of Molecular Modeling and Simulation: Select Papers from FOMMS 2015", Randall Q. Snurr, Claire S. Adjiman and David A. Kofke (Eds), Edward J. Maginn, series editor, Springer Singapore, 2016. DOI: 10.1007/978-981-10-1128-3

Refereed Archival Journal Publications - *Corresponding author underlined.* (Oct. 12, 2018 Google Scholar: 17,524 total citations, h-index = 64; Web of Science: 12,945 citations, h-index = 55).

1. E. J. Maginn, A. T. Bell, and D. N. Theodorou, "Transport Diffusivity of Methane in Silicalite from Equilibrium and Nonequilibrium Simulations", *Journal of Physical Chemistry,* **1993,** *97,* 4173-4181.
2. E. J. Maginn, A. T. Bell, and D. N. Theodorou, "Sorption Thermodynamics, Siting and Conformation of Long n-Alkanes in Silicalite as Predicted by Configurational-Bias Monte Carlo Integration", *Journal of Physical Chemistry*, **1995**, *99,* 2057-2079.
3. E. J. Maginn, A. T. Bell, D. N. Theodorou, "Dynamics of Long n-Alkanes in Silicalite: A Hierarchical Simulations Approach", *Journal of Physical Chemistry,* **1996**, *100,* 7155-7173.
4. R. Runnebaum and E. J. Maginn "Molecular Dynamics Simulations of Alkanes in the Zeolite Silicalite: Evidence for Resonant Diffusion Effects", *Journal of Physical Chemistry B,* **1997**, *101,* 6394-6408.
5. Y. N. Kaznessis, D. A. Hill and E. J. Maginn, "Molecular Dynamics Simulations of Polar Polymer Brushes", *Macromolecules,* **1998**, 31, 3116-3129.
6. Y. N. Kaznessis, D. A. Hill and E. J. Maginn, "A Molecular Dynamics Study of Macromolecules in Good Solvents: Comparison with Dielectric Spectroscopy Experiments", *Journal of Chemical Physics,* **1998**, 109, 5078-5088.
7. M. D. Macedonia and E. J. Maginn, "Pure and Binary Component Sorption Equilibria of Light Hydrocarbons in the Zeolite Silicalite from Grand Canonical Monte Carlo Simulations", *Fluid Phase Equilibria,* **1999**, 158-160, 19-27.
8. L. I. Kioupis and E. J. Maginn, "Rheology, Dynamics and Structure of Hydrocarbon Blends. A Molecular Dynamics Study of n-Hexane / n-Hexadecane Mixtures", *The Chemical Engineering Journal*, **1999**, 74, 129-146 (invited paper for special edition on molecular modeling).
9. Y. N. Kaznessis, D. A. Hill and E. J. Maginn, "Concentration and Size Dependence of Dielectric Strength and Dielectric Relaxation of Polymers in Solutions of a Theta Solvent via Molecular Dynamics Simulations", *Macromolecules,* **1999**, 32, 1284-1292.
10. M. D. Macedonia and E. J. Maginn, "A Biased Grand Canonical Monte Carlo Method for Simulating Adsorption Using All-Atom and Branched United Atom Models", *Molecular Physics*, **1999**, 96, 1375-1390.
11. Y. N. Kaznessis, D. A. Hill and E. J. Maginn, "Molecular Dynamics Simulations of Dielectric Relaxation of Concentrated Polymer Solutions", *Journal of Chemical Physics,* **1999**, 111, 1325-1334.
12. Y. N. Kaznessis, D. A. Hill and E. J. Maginn, "Dielectric Relaxation of Dipole-inverted Polar Polymers as Studied by Computer Simulations", *Macromolecules,* **1999**, 32, 6679-6686.
13. L. I. Kioupis and E. J. Maginn, "Molecular Simulation of Poly-alpha-olefin Synthetic

Lubricants: Impact of Molecular Architecture on Performance Properties", *Journal of Physical Chemistry B*, **1999**, 103, 10781-10790.

14. M. D. Macedonia, D. D. Moore, E. J. Maginn, and M. M. Olken, "Adsorption Studies of Methane, Ethane, and Argon in the Zeolite Mordenite: Molecular Simulations and Experiments", *Langmuir*, **2000**, 16, 3823-3834.
15. G. Arya, E. J. Maginn and H.-C. Chang, "Efficient Viscosity Estimation from Molecular Dynamics Simulation via Momentum Impulse Relaxation", *Journal of Chemical Physics*, **2000**, 113, 2079-2087.
16. M. D. Macedonia and E. J. Maginn, "Impact of Confinement on Zeolite Cracking Selectivity via Monte Carlo Integration", *AIChE Journal*, **2000**. 46, 2504-2517.
17. L. I. Kioupis and E. J. Maginn, "Impact of Molecular Architecture on the High-Pressure Rheology of Hydrocarbon Fluids", *Journal of Physical Chemistry B*, **2000**, 104, 7774-7783.
18. R. I. Nooney, M. Kalyanaraman, G. Kennedy, and E. J. Maginn, "Heavy Metal Remediation Using Functionalized Mesoporous Silicas with Controlled Macrostructure", *Langmuir*, **2001**, 17, 528-533.
19. G. Arya, E. J. Maginn and H. –C. Chang, "Effect of Surface Energy Barrier on Sorbate Diffusion in AlPO-5", *Journal of Physical Chemistry B*, **2001**. 105, 2725-2735.
20. G. Arya, H.-C. Chang, and E. J. Maginn, "A Critical Comparison of Equilibrium, Nonequilibrium and Boundary-Driven Molecular Dynamics Techniques for Studying Transport in Microporous Materials", *Journal of Chemical Physics*, **2001**, 115, 8112-8124.
21. J. L. Anthony, E. J. Maginn and J. F. Brennecke, "Solution Thermodynamics of Imidazolium-Based Ionic Liquids in Water", *Journal of Physical Chemistry B*, **2001**, 105, 10942-10949.
22. J. F. Brennecke and E. J. Maginn, "Ionic Liquids: Innovative Fluids for Chemical Processing" *AIChE Journal* **2001**, 47, 2384-2389 (invited "Perspectives" article).
23. L. I. Kioupis and E. J. Maginn, "Pressure-Enthalpy Driven Molecular Dynamics for Thermodynamic Property Calculation: I. Methodology", *Fluid Phase Equilibria*, **2002**, 200, 75-92.
24. L. I. Kioupis, G. Arya and E. J. Maginn, "Pressure-Enthalpy Driven Molecular Dynamics for Thermodynamic Property Calculation: II. Applications", F*luid Phase Equilibria*, **2002**, 200, 93-110.
25. J. Shah, J. F. Brennecke, and E. J. Maginn, "Thermodynamic Properties of the Ionic Liquid 1-n-butyl-3-methylimidazolium hexafluorophosphate from Monte Carlo Simulations", *Green Chemistry*, **2002**, 4, 112-118.
26. J. L. Anthony, E. J. Maginn and J. F. Brennecke, "Solubilities and Thermodynamic Properties of Gases in the Ionic Liquid 1-n-butyl-3-methylimidazolium hexafluorophosphate", *Journal of Physical Chemistry B.*, **2002,** 106, 7315-7320.
27. T. I. Morrow and E. J. Maginn, "Molecular Dynamics Study of the Ionic Liquid 1-n-butyl-3-methyl-imidazolium hexafluorophosphate", *Journal of Physical Chemistry B*, **2002**, 106, 12807-12813.
28. G. Arya, H. –C. Chang and E. J. Maginn, "Molecular Simulations of Knudsen Wall Slip: Effect of Wall Morphology", *Molecular Simulation*, **2003**, 29, 697-709.
29. G. Arya, H. –C. Chang and E. J. Maginn, "Knudsen Diffusivity of a Hard Sphere in a Rough Slit Pore", *Physical Review Letters*, **2003**, 91, 026102-1 – 026102-4.
30. D. Eike, J. F. Brennecke, and E. J. Maginn, "Predicting Melting Points of Quaternary Ammonium Ionic Liquids", *Green Chemistry*, **2003**, 5, 323-328.
31. Timothy I. Morrow, and Edward J. Maginn, correction to "Molecular Dynamics Study of the

Ionic Liquid 1-n-butyl-3-methyl-imidazolium hexafluorophosphate", *Journal of Physical Chemistry B*, **2003**, 107, 9160.

32. T. I. Morrow and E. J. Maginn, "Density, Local Composition and Diffusivity of Aqueous Choline Chloride Solutions: A Molecular Dynamics Study", *Fluid Phase Equilibria*, **2004**, 217, 97-104.
33. Jennifer L. Anthony, Sudhir N.V.K. Aki, Edward J. Maginn, and Joan F. Brennecke, "Feasibility of Using Ionic Liquids for Carbon Dioxide Capture," *International Journal of Environmental Technology and Management*, **2004,** 4, 105-115.
34. Jindal K. Shah and Edward J. Maginn, "A Monte Carlo Simulation Study of the Ionic Liquid 1-n-Butyl-3-Methylimidazolium Hexafluorophosphate: Liquid Structure, Volumetric Properties, and Infinite Dilution Solution Thermodynamics of CO_2", *Fluid Phase Equilibria*, **2004**, 222-223, 195-203.
35. Jacob M. Crosthwaite, Sudhir N. V. K. Aki, Edward J. Maginn and Joan F. Brennecke, "Liquid Phase Behavior of Imidazolium-Based Ionic Liquids with Alcohols", *Journal of Physical Chemistry B*, **2004**, 108, 5113-5119.
36. David Eike, Joan F. Brennecke, and Edward J. Maginn, "Predicting Infinite-Dilution Activity Coefficients of Organic Solutes in Ionic Liquids", *Industrial and Engineering Chemistry Research*, **2004**, 43, 1039-1048**.**
37. Cesar Cadena, Jennifer L. Anthony, Jindal K. Shah, Timothy I. Morrow, Joan F. Brennecke and Edward J. Maginn, "Why is CO_2 So Soluble in Imidazolium-based Ionic Liquids?", *Journal of the American Chemical Society*, **2004**, 126, 5300-5308.
38. James P. Larentzos, Abraham Clearfield, Akilesh Tripathi and Edward J. Maginn, "A Molecular Modeling Investigation of Cation and Water Siting in Crystalline Silicotitanates", *Journal of Physical Chemistry B*, **2004**, 108, 17560-17570.
39. David M. Eike, Joan F. Brennecke, and Edward J. Maginn, "Toward a Robust and General Molecular Simulation Method for Computing Solid-Liquid Coexistence", *Journal of Chemical Physics*, **2005**, 122, 014115-1 – 014115-12.
40. François Bonhomme, James P. Larentzos, Todd M. Alam, Edward J. Maginn and May Nyman, "Synthesis, Structural Characterization, and Molecular Modeling of Dodecaniobate Keggin Chain Materials", *Inorganic Chemistry*, **2005**, 44, 1774-1785.
41. Timothy I. Morrow and Edward J. Maginn, "Isomolar Semigrand Ensemble Molecular Dynamics: Development and Application to Liquid-Liquid Equilibria", *Journal of Chemical Physics*, **2005**, 122, 054504-1 – 054504-17.
42. Jennifer L. Anthony, Jessica L. Anderson, Edward J. Maginn and Joan F. Brennecke, "Anion Effects on Gas Solubility in Ionic Liquids", *Journal of Physical Chemistry B*, **2005**, 109, 6366-6374.
43. Jindal K. Shah and Edward J. Maginn, "Monte Carlo Simulations of Gas Solubility in the Ionic Liquid 1-*n*-butyl-3-methylimidazolium hexafluorophosphate", *J. Physical Chemistry B.*, **2005**, 109, 10395-10405.
44. J. M. Crosthwaite, S. N. V. K. Aki, E. J. Maginn and J. F. Brennecke, "Liquid Phase Behavior of Imidazolium-Based Ionic Liquids with Alcohols: Effect of Hydrogen Bonding and Non-Polar Interactions", *Fluid Phase Equilibria*, **2005**, 228, 303-309.
45. Manish S. Kelkar and Edward J. Maginn, "Rapid Shear Viscosity Calculation by Momentum Impulse Relaxation Molecular Dynamics", *Journal Chemical Physics*, **2005**, 123, 224904.
46. David J. Couling, Randall J. Bernot, Kathryn M. Docherty, JaNeille K. Dixon, and Edward J. Maginn, "Assessing the factors responsible for ionic liquid toxicity to aquatic organisms *via*

quantitative structure-property relationship modeling", *Green Chemistry*, **2006**, 8, 82-90.

47. Cesar Cadena, Qi. Zhao, Randall Q. Snurr and Edward J. Maginn, "Molecular Modeling and Experimental Studies of the Thermodynamic and Transport Properties of Pyridinium-Based Ionic Liquids", *Journal of Physical Chemistry B.*, **2006**, 110, 2821-2832.
48. David M. Eike and Edward J. Maginn, "Atomistic Simulation of Solid-Liquid Coexistence for Molecular Systems: Application to Triazole and Benzene", *Journal of Chemical Physics*, **2006**, 124, 164503.
49. J. M. Crosthwaite, M. J. Muldoon, S. N. V. K. Aki, E. J. Maginn and J. F. Brennecke, "Liquid phase behavior of ionic liquids with alcohols: Experimental studies and modeling", *Journal of Physical Chemistry B*, **2006**, 110, 9354-9361.
50. Jessica L. Anderson, JaNeille K. Dixon, Edward J. Maginn and Joan F. Brennecke, "Measurement of SO_2 Solubility in Ionic Liquids", *Journal of Physical Chemistry B.*, **2006**, 110, 15059-15062.
51. C. Cadena and E. J. Maginn, "Molecular Simulation Study of Some Thermophysical and Transport Properties of Triazolium-based Ionic Liquids", *Journal of Physical Chemistry B*, **2006**, 110, 18026-18039.
52. T. I. Morrow and E. J. Maginn, "Isomolar-semigrand Ensemble Molecular Dynamics: Application to Vapor-liquid Equilibrium of the Mixture Methane/Ethane", *Journal of Chemical Physics*, **2006**, 125, 204712.
53. Q. Dai, D. Menzies, Q. Wang, A. E. Ostafin, S. N. Brown, D. Meisel, and E. J. Maginn, "Monitoring the Synthesis and Composition Analysis of Microsilica Encapsulated Acetylacetonatacarbonyltriphenylphosphinerhodium Catalyst by Inductively Coupled Plasma (ICP) Techniques", *IEEE Transactions on Nanotechnology*, **2006**, 5, 677-682.
54. B. R. Novak, E. J. Maginn and M. J. McCready, "Comparison of Heterogeneous and Homogeneous Bubble Nucleation using Molecular Simulations", *Physical Review B*, **2007**, 75, 085413.
55. May Nyman, James P. Larentzos, Edward J. Maginn, Margaret E. Welk, David Ingersoll, Hyunsoo Park, John B. Parise, Ivor Bull, and François Bonhomme, "Experimental and Theoretical Methods to Investigate Extraframework Species in a Layered Material of Dodecaniobate Anions", *Inorganic Chemistry*, **2007**, *46*(6) pp 2067 – 2079.
56. Daniel Strasser, Fabien Goulay, Manish S. Kelkar, Edward J. Maginn and Stephen R. Leone, "Photoelectron Spectrum of Isolated Ion-Pairs in Ionic Liquid Vapor", *Journal of Physical Chemistry A*, **2007**, 111, 3191-3195.
57. Manish S. Kelkar and Edward J. Maginn, "Effect of Temperature and Water Content on the Shear Viscosity of the Ionic Liquid 1-ethyl-3-methylimidazolium Bis(trifluoromethanesulfonyl)imide As Studied by Atomistic Simulations", *Journal of Physical Chemistry B*, **2007**, 111, 4867-4876.
58. Wei Shi and Edward J. Maginn, "Continuous Fractional Component Monte Carlo: An Adaptive Biasing Method for Open System Atomistic Simulations", *Journal of Chemical Theory and Computation*, **2007**, 3, 1451-1463.
59. James Larentzos, William F. Schneider and Edward J. Maginn, "A Transferable Force Field for Water Adsorption in Cation Exchanged Titanosilicates", *Industrial and Engineering Chemistry Research*, **2007**, 46, 5754-5765.
60. Manish S. Kelkar, Jake L. Rafferty, Edward J. Maginn and J. Ilja Siepmann, "Prediction of Viscosities and Vapor-Liquid Equilibria for Five Polyhydric Alcohols by Molecular Simulation", *Fluid Phase Equilibria*, **2007**, 260, 218-231.

61. Manish S. Kelkar and Edward J. Maginn, "Calculating the Enthalpy of Vaporization of Ionic Liquid Clusters", *Journal of Physical Chemistry B.*, **2007**, 111, 9424-9427.
62. Edward J. Maginn, "Atomistic Simulation of the Thermodynamic and Transport Properties of Ionic Liquids", invited article for *Accounts of Chemical Research*, **2007**, 40, 1200-1207.
63. Saivenkataraman Jayaraman and Edward J. Maginn, "Computing the Melting Point and Thermodynamic Stability of the Orthorhombic and Monoclinic Polymorphs of the Ionic Liquid 1-n-Butyl-3-methylimidazolium Chloride", *Journal of Chemical Physics*, **2007**, 127, 214504.
64. Wei Shi and Edward J. Maginn, "Atomistic Simulation of the Absorption of Carbon Dioxide and Water in the Ionic Liquid 1-n-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide ([hmim][Tf2N])", *Journal of Physical Chemistry B*, **2008**, 112, 2045-2055.
65. Brian Novak, Edward J. Maginn and Mark J. McCready, "An Atomistic Simulation Study of the Role of Asperities and Indentations on Heterogeneous Bubble Nucleation", *Journal of Heat Transfer - Transactions of the ASME*, **2008**, 130, 042411.
66. James Larentzos, Craig Powers and Edward J. Maginn, "Atomistic Simulation of Water Adsorption and Cation Siting in Polyoxoniobate Materials", *Microporous and Mesoporous Materials*, **2008**, 116, 532-539.
67. May Nyman, Craig R. Powers, Francois Bonhomme, Todd M. Alam, Edward J. Maginn, and David T. Hobbs, "Ion Exchange Behavior of One-Dimensional Linked Dodecaniobate Keggin Ion Materials", *Chemistry of Materials*, **2008**, 20(7), 2513-2521.
68. Wei Shi and Edward J. Maginn, "Improvement in Molecule Exchange Efficiency in Gibbs Ensemble Monte Carlo: Development and Implementation of the Continuous Fractional Component Move", *Journal of Computational Chemistry*, **2008**, 29, 2520-2530.
69. Christina Myers, Henry Pennline, David Luebke, Jeffery Ilconich, JaNeille Dixon, Edward J. Maginn and Joan F. Brennecke, "High Temperature Separation of Carbon Dioxide / Hydrogen Mixtures Using Facilitated Supported Liquid Membranes", *Journal of Membrane Science*, **2008**, 322, 28-31.
70. Keith Gutowski and Edward J. Maginn, "Amine-Functionalized Task-Specific Ionic Liquids: A Mechanistic Explanation for the Dramatic Increase in Viscosity Upon Complexation with CO_2 from Molecular Simulation", *Journal of the American Chemical Society*, **2008**, 130, 14690-14704.
71. Manish S. Kelkar, Wei Shi and Edward J. Maginn, "Determining the Accuracy of Classical Force Fields for Ionic Liquids: Atomistic Simulation of the Thermodynamic and Transport Properties of 1-Ethyl-3-methylimidazolium Ethylsulfate (]emim][EtSO4]) and Its Mixtures with Water", *Industrial and Engineering Chemistry Research*, **2008**, 47, 9115-9126.
72. Wei Shi and Edward J. Maginn, Molecular Simulation and Regular Solution Theory Modeling of Pure and Mixed Gas Absorption in the Ionic Liquids 1-n-Hexyl-3-methylimidazolium Bis(Trifluoromethylsulfonyl)amide ([hmim][Tf2N]), *Journal of Physical Chemistry B*, **2008**, 112, 16710-16720.
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74. Keith E. Gutowski, Burcu Gurkan and Edward J. Maginn, "Force Field for the Atomistic Simulation of the Properties of Hydrazine, Organic Hydrazine Derivatives, and Energetic Hydrizinium Ionic Liquids", *Pure and Applied Chemistry*, **2009**, 81, 1799-1828.

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77. Amrish Menjoge, JaNeille Dixon, Joan Brennecke, Edward Maginn and Sergey Vasenkov, "Influence of Water on Diffusion in Imidazolium-Based Ionic Liquids: A Pulsed Field Gradient NMR Study", *Journal of Physical Chemistry B*, **2009**, 113, 6353-6359.
78. Edward J. Maginn "From Discovery to Data: What Must Happen for Molecular Simulation to Become a Mainstream Chemical Engineering Tool", invited "Perspectives" article, *AIChE Journal*, **2009**, 55, 1304-1310.
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81. Edward J. Maginn, "Molecular Simulation of Ionic Liquids: Current Status and Future Opportunities", Invited review, *Journal of Physics: Condensed Matter*, **2009**, 21, 373101.
82. Gabriele Raabe and Edward J. Maginn, "Molecular Modeling of the Vapor-Liquid Equilibrium Properties of the Alternative Refrigerant 2,3,3,3-Tetrafluoro-1-propene (HFO-1234yf)", *Journal of Physical Chemistry Letters*, **2010**, 1, 93-96.
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85. Saivenkataraman Jayaraman, Aidan P. Thompson, Anatole von Lilienfeld, and Edward J. Maginn, "Molecular Simulation of the Thermal and Transport Properties of Three Alkali Nitrate Salts", *Industrial and Engineering Chemistry Research*, **2010**, 49, 559-571.
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87. Jindal K. Shah and Edward J. Maginn, "Molecular Dynamics Investigation of Biomimetic Ionic Liquids", *Fluid Phase Equilibria*, **2010**, 294, 197-205.
88. Hongjun Liu, Yingxi Zhu and Edward J. Maginn, "Molecular Simulation of Polyelectrolyte Conformational Dynamics Under an AC Electric Field", *Macromolecules*, **2010**, 43, 4805-4813.
89. Christopher Jones and Edward J. Maginn, "Materials and Processes for Carbon Capture and Sequestration", Guest Editorial for special issue on carbon capture and sequestration,

ChemSusChem, **2010**, 3: 863–864. doi: 10.1002/cssc.201000235.

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Invited Lectures and Addresses

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3. "Understanding Sorption and Diffusion in Microporous Materials Through Molecular Simulation", Department of Chemical Engineering, Auburn University, Auburn, AL, Feb. 26, **1997**.
4. "Development of Advanced Molecular Simulation Tools for Examining Sorption and Diffusion in Microporous Materials", Dow Chemical Company, Midland, MI, Mar 11, **1997**.
5. "Understanding Sorption and Diffusion in Microporous Materials Through Molecular Simulation", Midwest Thermodynamics and Statistical Mechanics Conference, George Williams College, Williams Bay, WI, May 16, **1997**.
6. "Predicting Thermodynamic and Transport Properties of Engineering Materials from Molecular Simulations", University of Notre Dame Physical Chemistry Seminar Series, Notre Dame, IN, Dec. 4, **1997**.
7. "Molecular Simulation of Complex Molecule Sorption and Diffusion in Microporous Materials", Molecular Simulations, Inc., San Diego, CA, Jan. 9, **1998**.

8. “Fundamental Studies of Sorption and Diffusion in Microporous Materials”, The BOC Group Technical Center, Murray Hill, NJ, Jan. 27, **1998**.
9. “Molecular Simulations of Polar Polymers: Brushes and Solutions”, Department of Chemistry Macromolecules Seminar, University of Wisconsin, Madison, WI, April 6, **1998**.
10. “Molecular-Level Investigation of the Thermodynamic and Transport Properties of Confined Fluids”, Department of Chemical Engineering, University of Pennsylvania, Philadelphia, PA, Oct. 4, **1998**.
11. “Configurational-bias Grand Canonical Monte Carlo Simulation of Hydrocarbon Sorption in Zeolites”, Catalysis and Sorption Consortium Meeting, Molecular Simulations, Inc., San Diego, CA, Nov. 4, **1998**.
12. “Molecular Simulation of Complex Molecules in Zeolites”, International Symposium on Molecular Simulation of Catalysts and Catalytic Processes, Spring American Chemical Society Meeting, Anaheim, CA, March, **1999**.
13. “Molecular Modeling as a Design Tool for Complex Systems: From Zeolite Catalysts to Synthetic Lubricants”, Mobil Technology Company, Strategic Technology Center, Paulsboro, NJ, May 19, **1999**.
14. “Can Molecular Simulations Be Used to Design Catalysts and Adsorbents?”, International Conference on Rational Approaches to New Materials Design and Synthesis, Philadelphia, PA, May 21, **1999**.
15. “Molecular Modeling and Experimental Studies of Mixed Gas Sorption in Zeolites”, Gordon Research Conference on Zeolitic and Layered Materials, Plymouth State College, Plymouth, NH, June 16, **1999**.
16. “Comparison of All-atom and United-atom Models for Simulating Sorption and Diffusion in Zeolites”, Centre Europeen de Calcul Atomique et Moleculaire (European Center for Atomic and Molecular Computations), Ecole Normale Superieure de Lyon, Lyon, France, Oct. 4-8, **1999**.
17. "Molecular Modeling and Theory of Binary Adsorption in Zeolites: What Works, What Doesn't and What Needs to be Done", Gordon Conference on Separations, Aug. 2000.
18. “Molecular Simulation as a Design Tool in Chemical Engineering”, Department of Chemical Engineering, University of Washington, Seattle, WA, Oct. 2, **2000**.
19. “Pressure-Enthalpy Driven Molecular Dynamics: A Simple and Efficient Method for Thermodynamic State Point Sampling”, Spring American Chemical Society Meeting, San Diego, CA, April **2001**.
20. “Molecular Dynamics Methods for Quantitative Thermophysical Property Calculation”, NIST Workshop on Molecular Modeling, Gaithersburg, MD, June, **2001**.
21. “Thermophysical Properties from Molecular Simulation: Methods, Applications and Insight”. Department of Chemical Engineering, Georgia Institute of Technology, Atlanta, GA, Oct. 10, **2001**.
22. “Thermophysical Properties from Molecular Simulation: Methods, Applications and Insight”. Department of Chemical Engineering, Brigham Young University, Provo, UT, Oct. 25, **2001**.
23. “Teaching Graduate Molecular Modeling and Theory: Past Experiences and New Directions”, AIChE National Meeting, Reno, NV, November **2001**.

24. "Characterization and Application of Room Temperature Ionic Liquids for "Green" Chemical Processing". Department of Chemical Engineering, University of California at Los Angeles, Los Angeles, CA, May 3, **2002**.
25. "Molecular Simulation of Fluid Wall Slip in Nanopores", American Chemical Society Great Lakes Regional Meeting, Minneapolis, MN, June 3, **2002**.
26. "Molecular Modeling of Ionic Liquid / Gas Mixtures", American Chemical Society Fall Meeting, Boston, MA, August 19, **2002**.
27. "In Search of Environmentally Benign Solvents: Are Ionic Liquids the Right Solution?" Physical Chemistry Seminar, Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN, September 5, **2002**.
28. "Molecular Simulation of Fluids in Nanopores" Yangtze Conference on Fluids and Interfaces, Nanjing – Choingqing, China, October 12-18, **2002**.
29. "Molecular Simulation of Wall Slip in Confined Fluids", Rheology Research Center, University of Wisconsin, Madison, WI, October 25, **2002**.
30. "Molecular Modeling of Room Temperature Ionic Liquids", Air Force Office of Scientific Research Workshop on Energetic Ionic Liquids, The Executive Conference and Training Center, Dulles, VA, October 9, **2002**.
31. "Computing the Viscosity of Hydrocarbon / Alcohol Mixtures", NIST Fluid Properties Challenge, American Institute of Chemical Engineers Meeting, Indianapolis, IN November 3, **2002**.
32. "In Search of Environmentally Benign Solvents: Are Ionic Liquids the Right Solution?", NDEER Symposium, University of Notre Dame, Notre Dame, IN November 13, **2002**.
33. "In Search of Environmentally Benign Solvents: Are Ionic Liquids the Right Solution?", Department of Chemical Engineering, Princeton University, Princeton, NJ, December 11, **2002**.
34. "In Search of Environmentally Benign Solvents: Are Ionic Liquids the Right Solution?", Department of Chemical Engineering, State University of New York, Buffalo, NY, Februrary 19, **2003**.
35. "Molecular Modeling of the Thermodynamic and Transport Properties of Ionic Liquids", 226th ACS Meeting, New York, September 7, **2003**.
36. "Molecular Modeling of the Thermodynamic and Transport Properties of Industrially-Relevant Fluids: Methods, Results and Insights", 226th ACS Meeting, New York, September 10, **2003**.
37. "Molecular Simulation of Ionic Liquids: Thermodynamic Properties and Phase Behavior", Université Blaise Pascal, Clermont-Ferrand, France, September 30, **2003**.
38. "The Importance of Wall Slip on Diffusion in the Knudsen Regime", Centre Européen de Calcul Atomique et Moléculaire (CECAM) workshop, Ecole Normale Supérieure, Lyon, France, October 3, **2003**.
39. "Molecular Modeling of Thermodynamic and Transport Properties of Fluids: Methods, Results and Insights", Department of Chemical Engineering, University of Tennessee, Knoxville, TN October 21, **2003**.
40. "Molecular Modeling of Thermodynamic and Transport Properties of Fluids: Methods, Results and Insights", Department of Chemical Engineering, University of Massachusetts, Amherst, MA, October 23, **2003**.
41. "Design and Evaluation of Ionic Liquids as Novel CO_2 Absorbents", National Energy Technology Laboratory, Pittsburgh, PA, August 18, **2004**.

42. North American Lectures in Chemical Engineering: "In Search of Environmentally Benign Solvents: Are Ionic Liquids the Right Solution?" Instituto Mexicano del Petróleo, Mexico City, Mexico, October 22, 2004; "Development of New Molecular Dynamics Sampling Methods for Phase Equilibria Calculations", Department of Physics, Universidad Nacional Autónoma de México, Mexico City, Mexico, October 23, **2004**.
43. "Environmentally Benign Solvents for Reactions and Separations: Are Ionic Liquids the Right Solution?", Environmental Science, Engineering and Policy in the 21st Century Seminar Series, Environmental and Water Resources Engineering Program, University of Michigan, Ann Arbor, MI, January 28, **2005**.
44. "That's a Salt? The Properties and Potential Uses of Ionic Liquids", Department of Chemical and Biomolecular Engineering, Tulane University, March 4, **2005**.
45. "Determining Thermophysical Properties of New Materials via Molecular Modeling", Northwest Indiana Computational Grid Workshop, Purdue University, West Lafayette, IN, March 8, **2005**.
46. "Development of New Molecular Dynamics Sampling Methods for Phase Equilibria Calculations", Department of Chemical Engineering, Carnegie-Mellon University, March 17, **2005**.
47. "In Search of Environmentally Benign Solvents: Are Ionic Liquids the Right Solution?", Department of Chemical and Petroleum Engineering, University of Pittsburgh, March 18, **2005**.
48. "That's a Salt? The Properties and Potential Uses of Ionic Liquids", Department of Chemical Engineering, Texas Tech University, April 1, **2005**.
49. "In Search of Environmentally Benign Solvents: Are Ionic Liquids the Right Solution?", Department of Chemical Engineering, Colorado School of Mines, April 22, **2005**.
50. "Molecular Simulation of Ionic Liquids", Air Force Office of Scientific Research Contractor's Meeting in Molecular Dynamics, Monterey, CA, May 23, **2005**.
51. "Thermodynamic and Transport Properties of Ionic Liquids: Experiments and Atomistic Simulations", Faculty of Engineering Sciences, Friedrich-Alexander-Universität, Erlangen, Germany, June 24, **2005**.
52. "Atomistic Simulations of Ionic Liquids: Making the Link Between Structure and Properties", Department of Chemistry seminar, University of Iowa, Iowa City, IA, September 9, **2005**.
53. "Development and Application of Atomistic Simulations to the Study of New Materials: From Ionic Liquids to Crystalline Nanoporous Adsorbents", UOP Research Center, Des Plaines, IL, Sept. 29, **2005**.
54. "Development of New Molecular Dynamics Sampling Methods for Phase Equilibria Calculations", China / USA / Japan Joint Chemical Engineering Conference, Beijing, China, October 13, **2005**.
55. "Cool Molten Salts: The Interesting (and Potentially Useful) Properties of Ionic Liquids", Chemical Engineering departmental seminar, Vanderbilt University, March 13, **2006**.
56. "Modeling, Properties and Toxicology of Ionic Liquids", Ionic Liquids Workshop "Background, State-of-the-Art and Academic/Industrial Applications", University of Alabama, March 23, **2006**.
57. "Atomistic Simulation of Ionic Liquids Containing Pyridinium and Triazolium Cations", Spring 2006 National ACS Meeting, Symposium on Ionic Liquids, Atlanta, GA, March 26, **2006**.

58. "Atomistic Simulation of Ionic Systems: Application to Ionic Liquids and Nanoporous Ion Exchangers", Chemical Engineering departmental seminar, Purdue University, West Lafayette, IN, March 28, **2006**.
59. "Atomistic Simulation of Ionic Systems: Application to Ionic Liquids and Nanoporous Ion Exchangers", Department of Chemical and Petroleum Engineering seminar, University of Kansas, Lawrence, KS, April 11, **2006**.
60. "Atomistic Modeling of Adsorption and Ion Exchange in Zeolites", Plenary Lecture, 7th International Conference on the Occurrence, Properties and Utilization of Natural Zeolites, Socorro, NM, July 16-21, **2006**.
61. "Design and Evaluation of Ionic Liquids as Novel CO_2 Absorbents", National Energy Technology Program Review, Pittsburgh, PA, September 22, **2006**.
62. "Using Atomistic Simulations to Understand Structure-Property Relationships: Applications to Ionic Liquids and Crystalline Nanoporous Materials", Department of Chemistry and Department of Chemical and Biological Engineering, Iowa State University, Ames, IA, October 6, **2006**.
63. "Design and Evaluation of Ionic Liquids for Post-Combustion CO_2 Capture", American Filtration and Separation Society Annual Meeting, Pittsburgh, PA, Oct 16, **2006**.
64. "Using Atomistic Simulations to Understand Structure-Property Relationships: Application to Ionic Liquids and Crystalline Nanoporous Materials", Case Western Reserve University departmental seminar, November 9, **2006**.
65. "Using Atomistic Simulations to Understand Structure-Property Relationships: Application to Ionic Liquids and Crystalline Nanoporous Materials", Chemical and Biological Engineering seminar, University of Colorado, Boulder, CO, March 13, **2007**.
66. "Using Atomistic Simulations to Understand Structure-Property Relationships: Application to Ionic Liquids and Crystalline Nanoporous Materials", Chemical and Biological Engineering seminar, Northwestern University, Evanston, IL, March 29, **2007**.
67. "Can Classical Simulations Really Predict Properties of Ionic Liquids? On the Pitfalls and Success Stories of Modeling Ionic Liquids", Structures and Dynamics of Ionic Liquids conference, Kazusa Akademia Park, Chiba, Japan, August 3, **2007**.
68. "Using Atomistic Simulations to Predict the Thermodynamic and Transport Properties of Ionic Liquids", Second International Congress on Ionic Liquids, Yokohama, Japan, August 7, **2007**.
69. "Development and Use of Atomistic Simulation Methods to Understand Structure-Property Relationships for Ionic Liquids", Department of Chemical Engineering Colloquium, Rice University, Oct. 18, **2007**.
70. "Development of new post-combustion carbon dioxide capture solvents: Are ionic liquids the answer?" American Chemical Society meeting, New Orleans, LA, April 7, **2008**.
71. "Development and application of advanced molecular simulation methods for computing the properties of ionic liquids", American Institute of Chemical Engineers Spring Meeting, New Orleans, LA, April 8, **2008**.
72. "Development and Use of Atomistic Simulation Methods to Understand Structure-Property Relationships for Ionic Liquids", Department of Chemical, Biological and Materials Engineering, University of Oklahoma, April 24, **2008**.
73. "Is There Really an Energy Crisis?", University of Notre Dame College of Engineering Alumni Reunion Weekend, Notre Dame, IN, May 30, **2008**.

74. "The Development and Use of a Slow Growth Continuous Fractional Component Monte Carlo Move for Simulating Phase Behavior in Open Systems", ExxonMobil Corporate Research, Clinton, NJ, July 8, **2008**.
75. "On the Use of Atomistic Simulations to Understand and Predict the Thermodynamic Properties of Ionic Liquids" (Plenary Lecture), 20th International Conference on Chemical Thermodynamics, Warsaw, Poland, Aug. 3-8, **2008**.
76. "Carbon Dioxide Capture from Flue Gas Using Ionic Liquids: A Combined Molecular Modeling and Experimental Study" (Keynote Speaker), ASME 3rd Energy Nanotechnology International Conference, Jacksonville, FL, Aug. 10-14, **2008**.
77. "Contemporary Research Directions Related to Energy", Symposium of Undergraduate Research on Green Energy, University of Notre Dame, Oct. 1, **2008**.
78. "Molecular Modeling as a Tool for Relating Properties of Ionic Liquids to Chemical Structure", 214th Electrochemical Society Meeting, Honolulu, Hawaii, October 12, **2008**.
79. "Progress and Outlook for Molecular Dynamics Simulations", AIChE Centennial Session on Molecular Modeling, AIChE meeting, November 18, **2008**.
80. "Using Molecular Simulations to Design New Ionic Liquids for Use in Energy and Propulsion Applications", University of Florida Chemical Engineering departmental seminar, February 3, **2009**.
81. "Development of Technologies for Carbon Dioxide Capture", Michiana Area Engineers Week, February 28, **2009**.
82. "Development of Technologies for Carbon Dioxide Capture", American Society of Heating, Refrigeration and Air Conditioning Engineers, South Bend, IN, March 19, **2009**.
83. "Ionic Liquids" Breakthrough Absorption Technology for Post-Combustion CO_2 Capture", NETL CO_2 Capture Conference, Pittsburgh, PA, March 24, **2009**.
84. "On the Use of Molecular Simulations for Computing Thermodynamic and Transport Properties of Ionic Liquids", Centre Europeen de Calcul Atomique et Moleculaire workshop, Dublin, Ireland, April 6, **2009**.
85. "Using Molecular Simulations to Design New Ionic Liquids for Use in Energy and Propulsion Applications", Department of Chemistry seminar, University of New Orleans, New Orleans, LA, April 17, **2009**.
86. "Design and Evaluation of Ionic Liquids as Novel CO_2 Absorbents", National Energy Technology Laboratory, Pittsburgh, PA, April 30, **2009**.
87. "On the Use of Monte Carlo and Molecular Dynamics to Probe the Properties of Ionic Liquids", Air Force Office of Scientific Research Molecular Dynamics Contractors' Meeting, San Diego, CA, May 17, **2009**.
88. "Molecular Modeling of Solubility in Ionic Liquids", 8th World Congress on Chemical Engineering, Montreal, Quebec, Canada, August, **2009**.
89. "Developing New Ionic Liquids for CO_2 Capture: A Success Story for Thermodynamics and Computational Molecular Design", GE Global Research Symposium on Emissions and Aftertreatment, GE Global Research Center, Niskayuna, NY, Sept. 17, **2009**.
90. "Understanding Sorption and Diffusion in Ionic Liquids Via Molecular Simulation", Fakultät für Chemie und Mineralogie, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Leipzig, Germany, Nov. 30, 2009.
91. "On the Use of Molecular Simulations to Compute Ionic Liquid Phase Behavior", Winter School on Ionic Liquids, Warnemünde, Germany, Dec. 3, **2009**.

92. "Molecular Simulation Methods for Computing Thermodynamic and Transport Properties of Ionic Liquids and Molten Salts", Eduard-Zintl-Institut für Anorganische und Physikalische, Chemie Technische Universität Darmstadt, Darmstadt, Germany, Dec. 7, **2009**.
93. "Development of Advanced Monte Carlo Methods for Simulating Complex Molecular Systems", Applied and Computational Mathematics and Statistics Colloquium, University of Notre Dame, March 15, **2010**.
94. "Understanding the behavior of chemically functionalized ionic liquids via molecular simulation", 239th American Chemical Society National Meeting, San Francisco, CA, March 21, **2010**.
95. "A Molecular Simulation Study of the Structure and Dynamics of Chemically Functionalized Ionic Liquids", 8th Liblice Conference on the Statistical Mechanics of Liquids, Brno, Czech Republic, June 15, **2010**.
96. "Molecular Simulation and Its Role in Energy and Environmental Research", Notre Dame College of Engineering emeritus faculty luncheon, October **2010**.
97. "Tell Me Something I Don't Already Know: The Pivotal Role of Molecular Simulations in Ionic Liquids Discovery Research", Plenary Lecture, CoMSEF Session, AIChE National Meeting, Salt Lake City, UT, November, **2010**.
98. "Molecular Simulation and Its Role in Energy and Environmental Research", Indo-US Workshop on Energy and Environment: Challenges and Research Opportunities, Delhi, India, Dec. 12, **2010**.
99. "Developing New Materials for Energy and Environmental Applications Via Molecular Simulation", University of Pennsylvania Department of Chemical and Biomolecular Engineering, Philadelphia, PA, January 26, **2011**.
100. "Developing New Materials for Energy and Environmental Applications Via Molecular Simulation", National University of Singapore Department of Chemistry, Singapore, February 17, **2011**.
101. "Development of New Ionic Liquids Solvents for CO_2 Capture", National University of Singapore Department of Chemical Engineering, Singapore, February 18, **2011**.
102. "Developing New Materials for Energy and Environmental Applications Via Molecular Simulation" University of Minnesota Department of Chemical Engineering and Materials Science, Minneapolis, MN, March 29, **2011**.
103. "On the Use of Gradual Transformation Methods in Computing Phase Behavior", UCLA Institute for Pure and Applied Mathematics, Los Angeles, CA, May 17, **2011**.
104. "Criticality and Vapor-Liquid Phase Behavior of ionic liquids from Monte Carlo simulations", Air Force Office of Scientific Research Molecular Dynamics Program Meeting, Pasadena, CA, May 18, **2011**.
105. "How Molecular Simulations Can Save the World: Development of New Materials to Mitigate Greenhouse Gases", Vanderbilt University / Columbia University Molecular Modeling Cybercamp, Nashville, TN, June 3, **2011**.
106. "Criticality and Vapor-Liquid Phase Behavior of Ionic Liquids from Monte Carlo Simulations", Congress of Ionic Liquids (COIL) 4, Arlington, VA, June 18, **2011**.
107. "Criticality and Vapor-Liquid Phase Behavior of Ionic Liquids from Monte Carlo Simulations", Faraday Discussion 154: Ionic Liquids, Queen's University, Belfast, United Kingdom, August 23, **2011**.

108. "Developing New Materials for Energy and Environmental Applications Via Molecular Simulation", *Centennial Lecturer*, University of Alabama Chemical Engineering, Tuscaloosa, AL, Sept 22, **2011**.
109. "Criticality and Vapor-Liquid Phase Behavior of Ionic Liquids from Monte Carlo Simulations", Plenary speaker, XVIII International Conference on Chemical Thermodynamics in Russia, Samara, Russia, Oct. 5, **2011**.
110. "Developing New Materials for Energy and Environmental Applications Via Molecular Simulation", University of Washington Department of Chemical Engineering seminar, Seattle, WA, Nov. 14, **2011**.
111. "Developing New Materials for Energy and Environmental Applications Via Molecular Simulation", Louisiana State University Department of Chemical Engineering seminar, Baton Rouge, LA, January 20, **2012**.
112. "Using Molecular Simulation to Develop New Materials for Energy and Environmental Applications", Symposium on Chemical Physics of the Environment, Division of Chemical Physics of the American Physical Society, Boston, MA, Feb. 28, **2012**.
113. "Developing New Materials for Energy and Environmental Applications Via Molecular Simulation", MATGAS, Campus de la UAB, Bellaterra (Barcelona) – Spain, March 12, **2012**.
114. "Solubility and Interfacial Transport of CO_2 in Ionic Liquid Systems", ACS National Meeting, San Diego, CA, March 28, **2012**.
115. "Predicting Melting Points of Ionic Liquids Using Molecular Simulation", (Plenary lecture), Australasian Symposium on Ionic Liquids, Melbourne, Australia, May 4, **2012**.
116. "Water and Ionic Liquids: Solvation, Hydration and Other Curious Phenomena", Departmental Seminar, Materials Science and Engineering, Deakin University, Geelong, Australia, May 7, **2012**.
117. "Developing New Materials for Energy and Environmental Applications via Molecular Simulation", Department of Chemistry seminar, Monash University, Melbourne, Australia, May 8, **2012**.
118. "Predicting the Solubility Limits of Solids via Molecular Simulation", 2012 Workshop on Free Energy Methods in Drug Design (given by Andrew Paluch), Cambridge, MA, May 22, **2012**.
119. "Water and Ionic Liquids: Solvation, Hydration and Other Curious Phenomena", Department of Chemistry seminar, Queen's University, Belfast, Northern Ireland, May 31, **2012**.
120. "When Ionic Liquids Are Not Liquids: Simulating Vapor-Liquid and Solid-Liquid Phase Equilibrium of Ionic Liquids", (Plenary lecture), International Conference on Chemical Thermodynamics, Buzios, RJ, Brazil, August 5, **2012**.
121. "Leaping the Gap with ab initio Force Fields and Reactive Monte Carlo", Symposium on Bridging the Gap Between ab initio and Classical Simulations, American Chemical Society National Meeting, Philadelphia, PA, Aug. **2012**.
122. "Ionic Liquid Research at Notre Dame: Carbon Capture and Other Applications", The Future of Energy Forum, Trinity College, Dublin, Ireland August 30, **2012**.

123. "When Ionic Liquids Are Not Liquids: Simulating Vapor-Liquid and Solid-Liquid Phase Equilibrium of Ionic Liquids", invited plenary lecture, Equifase 2012, Puerto Varas, Chile, October 8, **2012**.
124. "What Can Molecular Modeling Tell Us About the Thermodynamics and Phase Behavior of Ionic Liquids", Department of Chemistry and Chemical Biology colloquium, Rutgers University, Piscataway, NJ, Dec. 11, **2012**.
125. "Application of Molecular Simulation to the Prediction of Ionic Liquid Properties", Workshop on Computational Chemistry and Materials, Argonne National Laboratory, Jan. 11, **2013**.
126. "Developing New Materials for Energy and Environmental Applications via Molecular Simulation", Department of Chemical Engineering colloquium, University of Illinois at Chicago, Chicago, IL March 7, **2013**.
127. "Developing New Materials for Energy and Environmental Applications via Molecular Simulation", Department of Chemical and Biological Engineering, Colorado School of Mines, Oct. 4, **2013**.
128. "An Engineer's View on Energy", Notre Dame Institute for Advanced Study, Oct. 29, **2013**.
129. "The Journey to Reliable Prediction of Thermophysical Properties Using Molecular Simulation: Are We There Yet?", Department of Chemical Engineering seminar, Imperial College London, London, England, Nov. 21, **2013**.
130. "Using Molecular Simulations to Develop Ionic Liquids with Tailored Properties", ExxonMobil Corporate Research and Development, Annandale, NJ, Dec. 12, **2013**.
131. "Force Field Comparison and Thermodynamic Property Calculation of Supercritical CO_2 and CH_4 Using Molecular Dynamics Simulations", American Chemical Society meeting, Dallas, TX, March 19, **2014**.
132. "A Computational Study of the Structure and Thermodynamic Properties of Solutions of Ionic Liquids and Dissolved Solutes", AFOSR Contractor Meeting, Arlington, VA, May 20, **2014**.
133. "Computing Solution Thermodynamics and Transport Properties of Ionic Liquids Mixed with Water and Organic Compounds", CECAM workshop "Multiscale Modelling of Ionic Liquids: From Quantum Methods to Coarse-Grained Models", EPFL, Lausanne, Switzerland, June 6, **2014**.
134. "A Computational Study of the Dynamics, Structure and Thermodynamic Properties of Water / Ionic Liquids Mixtures", Liquids 2014 Conference, Lisbon, Portugal, July 23, **2014**.
135. "The Journey to Reliable Prediction of Thermophysical Properties Using Molecular Simulation: Are We There Yet?", Amol Ajinkya Memorial Fund Lecture, Department of Chemical and Biological Engineering, University at Buffalo, Sept 10, **2014**.
136. "Development of Cassandra, an Integrated Monte Carlo Multi-Scale Molecular Modeling Platform for Materials Research", Software Institute for Molecular Simulations Workshop, Berkeley, CA, Sept 19, **2014**.
137. "Molecular Modeling Insights into the Mechanisms of Transport Property Trends in Ionic Liquids", AIChE Annual Meeting, special session in honor of Peter Cummings, Atlanta, GA, Nov. 17, **2014**.

138. "Predicting the Thermodynamic and Transport Properties of Ionic Liquids via Molecular Simulation", Department of Chemical and Biomolecular Engineering colloquium, University of California at Berkeley, Berkeley, CA, Feb. 25, **2015**.
139. "Using Molecular Simulation to Understand and Control the Thermodynamic and Transport Properties of Ionic Liquids", Department of Chemical Engineering colloquium, University of South Carolina, Columbia, SC. March 5, **2015**.
140. "Combining Molecular Simulations and Advanced Analysis Tools to Enable Rapid and Reliable Thermophysical Property Prediction", International Workshop on Molecular Modeling and Simulation: Science, Engineering and Industrial Applications, DECHEMA House, Frankfurt Main, Germany, March 24, **2015**.
141. "Using Molecular Simulation to Understand and Predict the Thermodynamic and Transport Properties of Ionic Liquids", Keynote Address, Foundations of Molecular Modeling and Simulation Welches, OR July 15, **2015**.
142. "How Dissolved Organic Molecules and Water Alter the Structure and Properties of Ionic Liquids: A Molecular Modeling Study", Joint European Molecular Liquid Group / Japanese Molecular Liquids Group annual meeting, Rostock. Germany, Sept. 9, **2015**.
143. "Using Molecular Simulation to Understand and Control the Thermodynamic and Transport Properties of Ionic Liquids", Department of Chemical and Biomolecular Engineering seminar, University of Maryland, College Park, MD, Sept. 22, **2015**.
144. "Molecular Modeling of the Thermodynamic and Transport Properties of Ionic Liquids: Can We Really Tell Experimentalists Anything", AIChE Area 1a Keynote Lecture, Salt Lake City, UT, Nov. 10, **2015**.
145. "Molecular Modeling of the Thermodynamic and Transport Properties of Ionic Liquids: Can We Really Tell Experimentalists Anything", Department of Chemical Engineering seminar, Tufts University, Medford, MA, Feb. 8 **2016**.
146. "Unraveling the Structure and Dynamics of Electrolytes and Ionic Liquids via Molecular Simulation", Department of Chemical and Biomolecular Engineering seminar, University of Houston, Sept 30, **2016**.
147. "Will Molecular Modeling Ever Become a Mainstream Chemical Engineering Tool", AIChE annual meeting, San Francisco, CA, Nov. 16, **2016**.
148. "Molecular Dynamics Simulations of U_{20} Nanoclusters and Ligand Binding", Materials Science of Actinides workshop, University of Notre Dame, Nov. 21, **2016**.
149. "Unraveling the Absorption Behavior and Structure of CO_2-Reactive Ionic Liquids via Molecular Simulation", Technical University of Delft Process Engineering and Energy Department colloquium, Delft, Netherlands, March 17, **2017**.
150. "Unraveling the Structure and Dynamics of Electrolytes and Ionic Liquids via Molecular Simulation", Department of Chemical, Biological and Materials Engineering colloquium, University of Oklahoma, Norman, OK April 19, **2017**.
151. "Cassandra: An Open Source Atomistic Monte Carlo Package for Materials Simulation", Scimeeting Europe: Materials Modeling and Simulation Conference, Athens, Greece, June 22, **2017**.
152. "Making Molecular Simulation a Reliable and Reproducible Tool", Keynote, Molecular Sciences Software Institute workshop on Developing Community Best Practices for Molecular Simulation Software, National Institute of Standards, Gaithersburg, MD, August 24, **2017**.

153. "Using Molecular Modeling to Design New Fluids for Energy Storage and Carbon Capture", Department of Chemical and Biomolecular Engineering colloquium, Lehigh University, Bethlehem, PA, Oct. 4, **2017**.
154. "Computational Design of New Materials for Energy Efficient Separations", Department of Chemical and Biomolecular Engineering colloquium, Clemson University, Clemson, SC, Oct. 26, **2017**.
155. "How to Use the Atomistic Monte Carlo Package Cassandra: Liquid Phase Properties and Vapor-Liquid Equilibria", special Computational Molecular Science and Engineering Forum Workshop, AIChE Annual Meeting, Minneapolis, MN, Oct. 30, **2017**.
156. "Computing Shear Viscosity Using Green-Kubo and Reverse Non-Equilibrium Molecular Dynamics: Best Practices and Caveats", Industrial Fluid Properties Simulation Challenge", AIChE Annual Meeting, Minneapolis, MN, Oct. 31, **2017**.
157. "Using Molecular Modeling to Design New Fluids for Energy Storage and Carbon Capture", Department of Chemical and Biomolecular Engineering colloquium, University of Michigan, Ann Arbor, MI, November 21, **2017**.
158. "Using Molecular Modeling to Design New Fluids for Energy Storage and Carbon Capture", Department of Chemical and Biological Engineering colloquium, University of Wisconsin, Madison, WI, December 5, **2017**.
159. "Computational Design of New Materials for Energy Efficient Separations", Department of Chemical and Petroleum Engineering colloquium, University of Pittsburgh, Pittsburgh, PA, Jan. 26, **2018**.
160. "Structure and Dynamics of Ionic Liquids from Atomistic Simulations", Department of Chemistry, Physical Chemistry Seminar, University of Rome Sapienza, Rome, Italy, March 14, **2018**.
161. "Computational Design of New Materials for Energy Efficient Separations", Department of Chemical and Environmental Engineering colloquium, University of California at Riverside, Riverside, CA, April 6, **2018**.
162. "Computational Design of New Materials for Energy Efficient Separations", Department of Chemical and Petroleum Engineering colloquium, University of Kansas, Lawrence, KS, April 10, **2018**.
163. "Using Reaction Ensemble Monte Carlo Simulations to Understand How Solvation and Confinement Affects Equilibrium Concentrations of Reacting Mixtures", Invited keynote, 8th International Symposium on Molecular Thermodynamics and Molecular Simulations, Narashino, Japan, September 5, **2018**.
164. "Molecular Modeling of Charged Systems: From Electrolytes to Ionic Liquids and Molten Salts", American Institute of Chemical Engineers Annual Meeting "New Frontiers in Molecular Thermodynamics", Oct. 30, **2018**.
165. "Computational Design of New Materials for Separations and Energy Storage", Department of Chemical Engineering, University of Texas, Auston, TX, Nov. 20, **2018**.

Other Lectures and Presentations - *Speaker underlined*

1. <u>G. R. Youngquist,</u> E. J. Maginn, and R. Lin, "Growth of Organic Crystals Under Nonuniform Conditions", AIChE Annual Meeting, Miami Beach, FL, November **1986**.

2. E. J. Maginn, A. T. Bell, and D. N. Theodorou, "Prediction of the Transport Diffusivity of Methane in Silicalite using Equilibrium and Nonequilibrium Simulation Techniques", AIChE Annual Meeting, Miami Beach, FL, November **1992.**
3. E. J. Maginn, A. T. Bell, and D. N. Theodorou, "Molecular Simulation of Hydrocarbon Sorption and Diffusion in Zeolites", 16th Annual Industrial Liason Program Conference, Berkeley, California, March **1994.**
4. E. J. Maginn, A. T. Bell, and D. N. Theodorou, "Low-Occupancy Sorption Thermodynamics of Long Alkanes in Silicalite Via Molecular Simulation", 10th International Zeolite Conference, Garmisch-Partenkirchen, Germany, July **1994.**
5. E. J. Maginn, A. T. Bell, and D. N. Theodorou, "Prediction of Sorption and Diffusion of Long-Chain Alkanes in Silicalite Through Systematic Coarse-Graining of Atomistic Models", AIChE Annual Meeting, San Francisco, CA, November **1994.**
6. E. J. Maginn, A. T. Bell, and D. N. Theodorou, "Molecular Simulation of Hydrocarbon Adsorption and Diffusion in Zeolites", Department of Chemical Engineering Colloquium, University of California, Berkeley, CA, January **1995.**
7. E. J. Maginn, A. T. Bell, and D. N. Theodorou, "A Hierarchical Simulation Approach to Predict the Diffusivity of Long-Chain Hydrocarbons in Zeolites", AIChE Annual Meeting, Miami Beach, FL, November 17, **1995.**
8. R. Runnebaum and E. J. Maginn, "Dynamics of Long *n*-Alkanes in Zeolites: A Mechanistic Study", 1996 Midwest Conference on Thermodynamics and Statistical Mechanics, Madison, WI, May 2, **1996.**
9. E. J. Maginn, R. Q. Snurr, A. T. Bell, D. N. Theodorou, "Simulation of Hydrocarbon Diffusion in Zeolites", 11th International Zeolite Conference, Seoul, Korea, August 13, **1996.**
10. R. Runnebaum and E. J. Maginn, "Dynamics of Long *n*-Alkanes in Zeolites: Evidence for Resonant Diffusion Effects", AIChE Annual Meeting, Chicago, IL, November 13, **1996.**
11. L. Gergidis, D. N. Theodorou, E. J. Maginn, A. T. Bell, "Prediction of Sorption and Diffusion of Hydrocarbons in Zeolites Through New, Hierarchical Simulation Techniques", 213th American Chemical Society National Meeting, San Francisco, CA, April 15, **1997.**
12. M. D. Macedonia, E. J. Maginn, J. Bicerano, and J. Garces, "General Simulation Tools to Study Multicomponent Sorption of Complex Molecules in Microporous Materials", AIChE Annual Meeting, Los Angeles, CA, November 19, **1997.**
13. Y. N. Kaznessis, E. J. Maginn and D. A. Hill, "Dielectric Relaxation of End-Grafted Polar Polymers via Molecular Dynamics Simulations", AIChE Annual Meeting, Los Angeles, CA, November 19, **1997.**
14. Y. N. Kaznessis, E. J. Maginn and D. A. Hill, "Dielectric Relaxation of Flexible Type-A Polar Macromolecules in Good Solvents", 1998 Midwest Conference on Thermodynamics and Statistical Mechanics, Notre Dame, IN, May 18, **1998.**
15. L. Kioupis, and E. J. Maginn, "Molecular Dynamics Studies of Hydrocarbon Mixtures", 1998 Midwest Conference on Thermodynamics and Statistical Mechanics, Notre Dame, IN, May 18, **1998.**
16. M. D. Macedonia and E. J. Maginn, "Grand Canonical Monte Carlo Simulation of Single Component and Binary Mixture Adsorption in Zeolites", 12th International Zeolite Conference, Baltimore, MD, July 7, **1998.**
17. E. J. Maginn, "Molecular Simulation and Experimental Investigation of Sorption in Zeolites", Third International Symposium on the Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids, Nicholas Copernicus University, Torun, Poland, Aug 9, **1998.**

18. M. D. Macedonia, and E. J. Maginn, "Monte Carlo Studies of Complex Sorbate Mixture Adsorption in Zeolites", AIChE Annual Meeting, Miami Beach, FL, Nov. 18, **1998**.
19. Y. N. Kaznessis, D. A. Hill and E. J. Maginn, "Molecular Dynamics Study of Dielectric Strength and Relaxation of Flexible Type-A Polar Macromolecules in Good and Theta Solvents", AIChE Annual Meeting, Miami Beach, FL, Nov. 19, **1998**.
20. L. I. Kioupis, and E. J. Maginn, "Molecular Dynamics Studies of Hydrocarbon Mixtures", AIChE Annual Meeting, Miami Beach, FL, Nov. 20, **1998**.
21. M. D. Macedonia, D. D. Moore, R. I. Nooney and E. J. Maginn, "Molecular Modeling and Experimental Studies of Mixed Gas Sorption in Zeolites", poster presentation, Gordon Research Conference on Zeolitic and Layered Materials, Plymouth State College, Plymouth, NH, June 13, **1999**.
22. L. I. Kioupis and E. J. Maginn, "Examining the Role of Molecule Architecture on Polyalphaolefin Lubricant Performance Using Molecular Simulation", AIChE Annual Meeting, Dallas, TX, Nov. 2, **1999**.
23. M. D. Macedonia, D. D. Moore, R. I. Nooney, and E. J. Maginn, "Molecular Modeling of Mixed Gas Sorption in Zeolites: The Role of Cations and Dealumination on Sorbate Siting and Selectivity", AIChE Annual Meeting, Dallas, TX, Nov. 3, **1999**.
24. Y. N. Kaznessis, D. A. Hill and E. J. Maginn, "Dielectric Relaxation of Dipole-Inverted Polar Polymers as Studied by Computer Simulations", AIChE Annual Meeting, Dallas, TX, Nov. 4, **1999**.
25. Nooney, R.I., Moore, D.D., Maginn, E.J., "Synthesis and Evaluation of Functionalized Mesoporous Silica Spheres for the Removal of Heavy Metals from Aqueous Streams and the Separation of Olefin-Paraffin Mixtures," ACS National Meeting, San Francisco, March **2000**.
26. G. Arya, E. J. Maginn and H. –C. Chang, "A Novel Approach to Calculating Shear Viscosity From Molecular Dynamics Simulations Via Momentum Impulse Relaxation", AIChE Annual Meeting, Los Angeles, November, **2000**.
27. R. I. Nooney, J. Shah and E. J. Maginn, "Functionalized Mesoporous Silicas With Controlled Macrostructure", AIChE Annual Meeting, Los Angeles, November **2000**.
28. R. W. Maier, E. J. Maginn and M. A. Stadtherr, "Reliable Density-Functional Theory Calculations of Adsorption in Nanoporous Materials", AIChE Annual Meeting, Los Angeles, November **2000**.
29. J. L. Anthony, E. J. Maginn and J. F. Brennecke, "Solution Thermodynamics of Imidazolium-Based Ionic Liquids and Water", Spring American Chemical Society Meeting, April **2001**.
30. J. L. Anthony, E. J. Maginn and J. F. Brennecke "Gas Solubility in Ionic Liquids", Spring American Chemical Society Meeting, April **2001**.
31. L. I. Kioupis and E. J. Maginn, "Understanding How Molecular Architecture Impacts the Performance Properties of Synthetic Lubricants Under Extreme Conditions via Molecular Simulation", Spring American Chemical Society Meeting, April **2001**.
32. R. I. Nooney and E. J. Maginn, "Adsorption in Functionalized Mesoporous Silica" (poster), 7th International Conference on Fundamentals of Adsorption, Nagasaki, Japan, May **2001**. (Won Best Poster award).
33. E. J. Maginn, "Fundamentals of Adsorption and Transport in Functionalized Mesoporous Materials", Molecular Devices Workshop, University of Notre Dame, July, **2001**.
34. G. Arya, H. –C. Chang and E. J. Maginn, "Effect of Surface Energy Barrier on Sorbate Diffusion in AlPO4-5", AIChE Annual Meeting, Reno, NV, November **2001**.

35. J. L. Anthony, J. F. Brennecke and E. J. Maginn, "Thermodynamics of Gases in Ionic Liquids", AIChE Annual Meeting, Reno, NV, November **2001**.
36. E. J. Maginn, L. I. Kioupis and G. Arya, "Pressure-Enthalpy Driven Molecular Dynamics for Thermodynamic Property Calculation", AIChE Annual Meeting, Reno, NV, November **2001**.
37. G. Arya, H. –C. Chang and E. J. Maginn, "A Critical Comparison of Equilibrium, Nonequilibrium and Boundary-Driven Molecular Dynamics Techniques for Studying Transport in Microporous Materials", AIChE Annual Meeting, Reno, NV, November **2001**.
38. J. L. Anthony, S. N. Aki, E. J. Maginn and J. F. Brennecke, "Carbon Dioxide Capture by Ionic Liquids", AIChE Annual Meeting, Indianapolis, IN, November, **2002**.
39. J. K. Shah, T. I. Morrow, J. F. Brennecke, and E. J. Maginn, "Thermodynamic Properties of Ionic Liquid / Gas Mixtures from Molecular Simulations", AIChE Annual Meeting, Indianapolis, IN, November, **2002**.
40. J. L. Anthony, S. N. Aki, E. J. Maginn and J. F. Brennecke, "Supported Ionic Liquid Membranes for Gas Separations", AIChE Annual Meeting, Indianapolis, IN, November, **2002**.
41. J. M. Crosthwaite, S. N. Aki, E. J. Maginn and J. F. Brennecke, "Liquid-Liquid Equilibria of Water and Organic Solvents in Ionic Liquids", AIChE Annual Meeting, Indianapolis, IN, November, **2002**.
42. G. Arya, H. –C. Chang, and E. J. Maginn, "Knudsen Slip for Gases in Micro- and Nano-channels: Effects of Wall Morphology and Inertia", AIChE Annual Meeting, Indianapolis, IN, November, **2002**.
43. S. N. V. K. Aki, J. M. Crosthwaite, J. L. Anthony, E. J. Maginn, and J. F. Brennecke, "Thermodynamics of Ionic Liquids for Separations", Fifteenth Symposium on Thermophysical Properties, Boulder, CO, June, **2003**.
44. E. J. Maginn, J. K. Shah and T. I. Morrow, "Molecular Modeling of Imidazolium-Based Ionic Liquids", Fifteenth Symposium on Thermophysical Properties, Boulder, CO, June, **2003**.
45. E. J. Maginn, J. K. Shah, T. I. Morrow, D. Eike and J. F. Brennecke, "Molecular Simulation of Ionic Liquids: Thermodynamic Properties and Phase Behavior", 2nd Conference on Foundations of Molecular Modeling and Simulation, Keystone, CO, July, **2003**.
46. J. L. Anthony, C. Cadena, E. J. Maginn and J. F. Brennecke "Effect of Ionic Liquid Structure on Gas Solubilities", 226th ACS Meeting, New York, September, **2003**.
47. J. K. Shah, J. L. Anthony, T. I. Morrow, J. F. Brennecke, and E. J. Maginn, "Monte Carlo Simulations of Gas Solubility in Ionic Liquids", 226th ACS Meeting, New York, September, **2003**.
48. T. I. Morrow and E. J. Maginn, "Short Time Local Dynamics of Ionic Liquids: Neutron Scattering and Molecular Dynamics Simulations", 226th ACS Meeting, New York, September, **2003**.
49. G. Arya, H. –C. Chang and E. J. Maginn, "Knudsen Diffusivity of a Hard Sphere in a Slit Pore", AIChE Annual Meeting, San Francisco, CA November, **2003**.
50. D. A. Kofke, R. L. Rowley and E. J. Maginn, "Molecular Simulation Modules for Instruction in Thermodynamics, Transport, Kinetics, and Materials", AIChE Annual Meeting, San Francisco, CA November, **2003**.
51. J. K. Shah and E. J. Maginn, "Monte Carlo Study of Volumetric Properties and Gas Solubility in the Ionic Liquid 1-n-butyl-3-methylimidazolium hexafluorophosphate", AIChE Annual Meeting, San Francisco, CA November, **2003**.

52. E. J. Maginn and J. Larentzos “"Molecular Modeling Investigation of Cation Siting in Crystalline Silicotitanate and Polyoxoniobate Materials", 227th ACS Meeting, Anaheim, CA, March, **2004**.
53. J. P. Larentzos and E. J. Maginn, Molecular Modeling of Ion Exchange in Crystalline Silicotitanate Materials”, 10th International Conference on Properties and Phase Equilibria for Product and Process Design”, Snowbird, UT, May, **2004**.
54. E. J. Maginn and J. P. Larentzos, “Molecular Modeling of the Ion Exchange Process in Crystalline Silicotitanate Materials for Cs, Sr, and Actinide Removal”, Plenary Lecture, 8th International Conference on the Fundamentals of Adsorption”, Sedona, AZ, May, **2004**.
55. Jennifer L. Anthony, Edward J. Maginn and Joan F. Brennecke, “How Ionic Liquid Structure Affects Gas Solubilities”, AIChE Annual meeting, Austin, TX, November **2004**.
56. Edward J. Maginn and James P. Larentzos, “Determination of Cation and Water Positions in Crystalline Silicotitanates and Polyoxoniobate Ion Exchange Materials”, AIChE Annual Meeting, Austin, TX, November **2004**.
57. David M. Eike and Edward J. Maginn, “Toward a Robust and General Molecular Dynamics Approach for Computing Solid-Liquid Equilibrium of Complex Molecular Systems”, AIChE Annual Meeting, Austin, TX, November **2004**.
58. Timothy I. Morrow and Edward J. Maginn, “Isomolar Semigrand Ensemble Molecular Dynamics: Development and Application to Liquid-Liquid Equilibria”, AIChE Annual Meeting, Austin, TX, November **2004**.
59. Edward J. Maginn, Brian R. Novak and Mark J. McCready, “Molecular Dynamics Simulation of Bubble Nucleation at a Patterned Solid Surface”, AIChE Annual meeting, Austin, TX, November **2004**.
60. Timothy I. Morrow and Edward J. Maginn, “Isomolar Semigrand Ensemble Molecular Dynamics: Application to Vapor-Liquid Equilibrium of the Mixture Methane/Ethane”, Midwest Thermodynamics and Statistical Mechanics Conference, West Lafayette, IN, May, **2005**.
61. Cesar Cadena and Edward J. Maginn, “Molecular Dynamics Study of Pyridinium- and Triazolium-Based Ionic Liquids”, Midwest Thermodynamics and Statistical Mechanics Conference, West Lafayette, IN, May **2005**.
62. Brian Novak, Mark McCready and Edward J. Maginn, “Superheated Homogeneous and Heterogeneous Bubble Nucleation Rates using NPT and $NP_{zz}T$ Moplecular Dynamics”, AIChE Annual Meeting, Cincinnati, OH, November, **2005**.
63. Cesar Cadena and Edward J. Maginn, “Molecular Dynamics Study of Pyridinium-Based Ionic Liquids”, AIChE Annual Meeting, Cincinnati, OH, November, **2005**.
64. David Eike and Edward J. Maginn, “Computing Solid-Fluid Coexistence for Molecular Systems Using a Pseudo-Supercritical Path Sampling Method”, AIChE Annual Meeting, Cincinnati, OH, November **2005**.
65. JaNeille K. Dixon, Mark Muldoon, Sudhir N.V.K. Aki, Jessica Anderson, Joan F. Brennecke, and Edward J. Maginn, “Tuning Ionic Liquids for CO_2 Gas Absorption”, AIChE Annual Meeting, Cincinnati, OH, November, **2005**.
66. Haizhong Zhang and Edward J. Maginn, “Modeling CO2 Solubility in Ionic Liquids Using Semi-Grand Canonical Ensemble Hybrid Monte Carlo”, AIChE Annual Meeting, Cincinnati, OH, November **2005**.

67. Jessica Anderson, JaNeille K. Dixon, Mark Muldoon, Edward J. Maginn, and Joan F. Brennecke, "Gas Solubilities in Tunable Ionic Liquids", AIChE Annual Meeting, Cincinnati, OH, November, **2005.**
68. Manish S. Kelkar and Edward J. Maginn, "Rapid Shear Viscosity Calculation by Momentum Impulse Relaxation Molecular Dynamics (MIR-MD)", AIChE Annual Meeting, Cincinnati, OH, November, **2005.**
69. Edward J. Maginn, "Atomistic Simulation of Pyridinium- and Triazolium-Based Ionic Liquids", 16th Symposium on Thermophysical Properties, Boulder, CO, July 30-Aug 4, **2006**.
70. Manish S. Kelkar and Edward J. Maginn, "Understanding the role of dissolved water on the properties of ionic liquids: An atomistic simulation study", AIChE Annual Meeting, San Francisco, CA, November, **2006**.
71. Brian Novak, Edward J. Maginn and Mark J. McCready, "Effects of Geometric Defects on Superheated Heterogeneous Bubble Nucleation: A Molecular Dynamics Study"**,** AIChE Annual Meeting, San Francisco, CA, November, **2006**.
72. Jessica L. Anderson, JaNeille K. Dixon, Edward J. Maginn, Joan F. Brennecke, "Ionic Liquids as Absorption Media for CO_2 Capture", AIChE Annual Meeting, San Francisco, CA, November, **2006**.
73. Joan Brennecke, Jessica L. Anderson, JaNeille K. Dixon, and Edward J. Maginn "Ionic Liquids for Post-Combustion CO2 Capture", AIChE Spring meeting, Houston, TX, April **2007**.
74. Craig Powers and Edward J. Maginn, "Influence of Water on N2/O2 Selectivity in Na-X Zeolite as Studied by Monte Carlo Simulations", Midwest Thermodynamics and Statistical Mechanics Conference, Iowa State University, June 7th, **2007**.
75. Saivekataraman Jayaraman and Edward J. Maginn, "Computing the Melting Point of Ionic Liquids from Atomistic Simulations", Midwest Thermodynamics and Statistical Mechanics Conference, Iowa State University, June 7th, **2007.**
76. Jessica Anderson, JaNeille. K. Dixon, Mark. J. Muldoon, J. F. Brenecke and Edward J. Maginn, "Ionic liquids as CO capture media", CHEMRAWN-XVII and ICCDU-IX Conference on Greenhouse Gases, Mitigation and Utilization, Kingston, Ontario, Canada, July 11, **2007**.
77. Brian Novak, Edward J. Maginn and Mark J. McCready, "Applying a Thermodynamic Model to Predict Bubble Nucleation", AIChE Annual Meeting, Salt Lake City, UT, Nov. **2007**.
78. Amrish R.Menjoge, JaNeille K. Dixon, Joan F. Brennekce, Edward J. Maginn, and Sergey Vasenkov, "Influence of Water on Diffusion in Ionic Liquids: Pulsed Field Gradient NMR Study", AIChE Annual Meeting, Salt Lake City, UT, Nov. **2007.**
79. Sai Jayaraman and Edward J. Maginn, "Computing the Melting Point of Ionic Liquids from Atomistic Simulations", AIChE Annual Meeting, Salt Lake City, UT, Nov. **2007**.
80. Wei Shi and Edward J. Maginn, "Continuous Fractional Component Monte Carlo: The General Biased Slow-Growth Method for Phase Equilibrium Simulations", AIChE Annual Meeting, Salt Lake City, UT, Nov. **2007**.
81. Jessica L. Anderson, JaNeille K. Dixon, Wei Shi, Kate E. Wilbanks, Edward J. Maginn and Joan F. Brennecke, "Ionic Liquids as Absorption Media for Mixed Gas Capture", AIChE Annual Meeting, Salt Lake City, UT, Nov. **2007**.
82. Edward J. Maginn, JaNeille K. Dixon, Elaine Mindrup, Wei Shi, Joan F. Brennecke, and William F. Schneider, "Evaluation of Ionic Liquids as Novel Post-Combustion Carbon

Dioxide Capture Solvents", American Institute of Chemical Engineers Spring Meeting, New Orlean, LA, April 8, **2008**.

83. Edward J. Maginn, "Evaluation of Ionic Liquids in Post-Combustion CO_2 Capture", Seventh Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA, May 6, **2008**.
84. Edward J. Maginn, Wei Shi, Keith Gutowski, Manish Kelkar and Saivenkataraman Jayaraman, "Development and Use of Atomistic Simulations to Understand Structure-Property Relationships for Ionic Liquids", Air Force Office of Scientific Research Contractors Meeting, Vienna, VA, May 20, **2008**.
85. Keith Gutowski and Edward J. Maginn, "Amine-Functionalized Task Specific Ionic Liquids for CO2 Capture", ACS Annual Meeting, Philadelphia, PA, August 20, **2008**.
86. Jindal Shah and Edward J. Maginn, "Novel Monte Carlo Algorithm to Sample Intramolecular Degrees of Freedom of Linear, Branched and Cyclic Molecules with Fixed Bond Length Constraints", AIChE Annual Meeting, Philadelphia, PA, November 19, **2008**.
87. Manish S. Kelkar and Edward J. Maginn, "On the Use of Molecular Modeling to Predict a Wide Range of Thermodynamic and Transport Properties of the Ionic Liquid 1-Ethyl-3-Methylimidazolium Ethylsulfate and Its Mixtures with Water", AIChE Annual Meeting, Philadelphia, PA, November 19, **2008**.
88. Manish S. Kelkar, Mark B. Shiflett, Akimichi Yokozeki and Edward J. Maginn, "Atomistic Simulation Study of Hydrofluorocarbon-Ionic Liquids Mixtures", AIChE Annual Meeting, Philadelphia, PA, November 19, **2008**.
89. Andrew Paluch, Sai Jayaraman, Jindal Shah and Edward J. Maginn, "An Adaptable Method to Calculate the Solubility Limit of Solids by Molecular Simulation", AIChE Annual Meeting, Nashville, TN, November 9, **2009.**
90. Craig M. Tenney and Edward J. Maginn, "Limitations and Recommendations for the Calculation of Shear Viscosity Using Reverse Nonequilibrium Molecular Dynamics", AIChE Annual Meeting, Nashville, TN, November 9, **2009.**
91. Marcos Perez-Blanco and Edward J. Maginn, "Molecular dynamics simulations of CO_2 at an ionic liquid interface: adsorption, ordering and interfacial crossing", AIChE Annual Meeting, Nashville, TN, November 12, **2009**.
92. Thomas Rosch, Wei Shi, Jindal Shah and Edward J. Maginn, "Improved Conformational Sampling for Reaction Ensemble Monte Carlo Simulations", AIChE Annual Meeting, Nashville, TN, November 12, **2009**.
93. Jindal Shah and Edward J. Maginn, Hydrophobic Type Interactions Between Ionic Liquids and Inorganic Salt Ions in Aqueous Environments: Molecular Dynamics Simulations", AIChE Annual Meeting, Nashville, TN, November 12, **2009**.
94. Edward Maginn, "Powering the Planet in a Carbon Constrained World", Hesburgh Lecture, Notre Dame Club of Sarasota, February 24, **2010**.
95. Gabriele Raabe and Edward J. Maginn, "A Force Field for Fluoropropenes, including HFO-1234yf", International Workshop "Molecular Modeling and Simulation for Industrial Application: Physico-chemical Properties and Processes", Würzburg, Germany, March, **2010**
96. Edward J. Maginn, Joan Brennecke, William Schneider and Mark McCready, "Molecular Engineering of New Ionic Liquid Sorbents for CO_2 Capture", 9th Annual Carbon Capture and Sequestration Meeting, Pittsburgh, PA, May 11, **2010**.
97. Jindal Shah and Edward J. Maginn, "Confinement Effects on Structure and Dynamics of Room Temperature Ionic Liquids: Molecular Dynamics Investigation", 12th International

Conference on Properties and Phase Equilibria for Product and Process Design, Suzhou, Jiangsu, China, May 16, **2010**.

98. Burcu E. Gurkan, Juan de la Fuente, Elaine M. Mindrup, Lindsay E. Ficke, Brett F. Goodrich, Erica A. Price, William F. Schneider, Edward J. Maginn and Joan F. Brennecke, "Chemically Complexing Ionic Liquids for Post-Combustion CO_2 Capture", Clearwater CCS Conference, Clearwater, FL, June 7, **2010**.
99. Andrew Paluch, David Mobley and Edward J. Maginn, "An Adaptable Method for Computing Solubilites of Complex Molecules", Midwest Thermodynamics and Statistical Mechanics Conference, University of Notre Dame, Notre Dame, IN, June 3, **2010**.
100. Hao Wu, Thomas Rosch, and Edward J. Maginn, "Understanding the Behavior of Chemically-Functionalized Ionic Liquids Via Molecular Simulation", ACS Annual National Meeting, Boston, MA, August, **2010**.
101. Marcos Perez-Blanco and Edward J. Maginn, "Molecular Dynamics Simulations of H_2O and CO_2 at An Ionic Liquid Interface: Effect of a Third Component On CO_2 Absorption Dynamics", AIChE Annual Meeting, Salt Lake City, UT, November 9, **2010**.
102. Hongjun Liu, Y. Elaine Zhu and Edward J. Maginn, "Molecular Simulation of Polyelectrolye Conformational Dynamics Under An AC Electric Field", AIChE Annual Meeting, Salt Lake City, UT, November 10, **2010**.
103. Thomas Rosch and Edward J. Maginn, "Predicting Carbon Dioxide Complexation in Ionic Liquids Using Reaction Ensemble Monte Carlo", AIChE Annual Meeting, Salt Lake City, UT, November 10, **2010**.
104. Neeraj Rai and Edward J. Maginn, "Computing Phase Behavior of Ionic Liquids Via Monte Carlo Simulations", AIChE Annual Meeting, Salt Lake City, UT, November 10, **2010**.
105. Andrew Paluch, Sai Jayaraman and Edward J. Maginn, "Predicting the Solubility Limit of Drug Molecules by Molecular Simulation", AIChE Annual Meeting, Salt Lake City, UT, November 11, **2010**.
106. Pavi Tiruppathi, Craig Tenney and Edward J. Maginn, "Molecular Simulation of Ionic Liquid Nanodroplets in Electric Fields", AIChE Annual Meeting, Salt Lake City, UT, November 11, **2010**.
107. Neeraj Rai and Edward J. Maginn, "Force Field Development for Uranyl Systems", ACS National Meeting, Anaheim, CA, March, **2011**.
108. Andrew Paluch and Edward J. Maginn, "Predicting the Solubility of Pharmaceutical Solids by Molecular Simulation", Gordon Research Conference on Computer Aided Drug Design, West Dover, VT, July, **2011**.
109. Neeraj Rai and Edward J. Maginn, "Force Field Development for Uranyl Systems via Electronic Structure Calculations", ACS National Meeting, Denver, CO, August 27, **2011**.
110. Gabriele Raabe and Edward J. Maginn, "Molecular Modeling of Alternative Fluoropropene Refrigerants, Including HFO-1234yf", Thermodynamics 2011, Athens, Greece, August 30, **2011**.
111. Jindal Shah, Patrick Yee and Edward J. Maginn, "Microscopic State of Ionic Liquid Ion Pairs At Low Concentrations In Water As Studied From Molecular Dynamics Simulations", AIChE Annual Meeting, Minneapolis, MN, October **2011**.
112. Jindal Shah and Edward J. Maginn, "Teaching Molecular Dynamics and Monte Carlo Simulations: Lessons Learned From the Statistical Thermodynamics Workshops At the School of Advanced Studies In Applied Thermodynamics, Rio De Janeiro, Brazil", AIChE Annual Meeting, Minneapolis, MN, October, **2011.**

113. Neeraj Rai, Surya P. Tiwari and Edward J. Maginn, "Developing Actinyl Force Field for Modeling Solvent Extraction Processes", 17th Symposium on Separation Science and Technology for Energy Applications", Gatlinburg, TN, October 23, **2011**.
114. Edward Maginn, "Powering the Planet in a Carbon Constrained World", Hesburgh Lecture for the Grand Rapids Area Notre Dame Club and Michigan Society of Civil Engineers, Grand Rapids, MI, January 4, **2012**.
115. Hongjun Liu and Edward J. Maginn, "Ion Shape Effect on Dynamics of Ionic Liquids", American Physical Society meeting, Boston, MA, Feb. 28, **2012**.
116. Yong Zhang and Edward J. Maginn, "Computing Melting Points of Ionic Liquids Using Molecular Simulations", ACS National Meeting, San Diego, CA, March 28, **2012**.
117. Yong Zhang, Marcos Perez-Blanco, and Edward J. Maginn, "Molecular Simulation of Ionic Liquids: Melting Points, Charge Distributions, and Interfacial Transport, Annual AFOSR Contractor's Meeting, Arlington, VA, May 22, **2012**.
118. Omar Abdelziz, Edward J. Maginn, and Doug Morrison, "Leading Edge Advances in Absorption Cooling Technologies", ASHRAE Winter Conference, Dallas Texas, Jan. 30, **2013**.
119. Edward Maginn, "Powering the Planet in a Carbon Constrained World", Hesburgh Lecture to the Central Pennsylvania Notre Dame Alumni Club and the College of Engineering, University of Pittsburgh at Johnstown, Johnstown, PA, Feb. 20, **2013**.
120. Katie Maerzke, William Schneider and Edward J. Maginn, "Molecular dynamics simulations of uranyl and plutonyl coordination in water/ionic liquid mixtures", ACS Annual Meeting, New Orleans, LA, April, **2013**.
121. Yong Zhang and Edward J. Maginn, "First Principle Prediction of Ionic Liquids Melting Points", Congress on Ionic Liquids, Vilamoura, Algarve, Portugal, April 24, **2013.**
122. Samir Budhathoki, Jindal K. Shah and Edward J. Maginn, "Molecular simulation study of the dynamics of ionic liquid (IL) [bmim][Tf2N] confined in graphite slit pore s", Congress on Ionic Liquids, Vilamoura, Algarve, Portugal, April 24, **2013**.
123. S. P. Verevkin, D. Zaitsau, A. V. Vermalayeu, V. N. Emel'yanenko, R. Ludwig, C. Schick, Y. Zhang and E. J. Maginn, "How a subsequent methylation of the imidazolium ring affects the thermochemical properties of ILs", Congress on Ionic Liquids, Vilamoura, Algarve, Portugal, April 24, **2013**.
124. J. F. Brennecke, E. J. Maginn, M. J. McCready, M. A. Stadtherr, W. F. Schneider, "Phase Change Ionic Liquids for Post-Combustion CO_2 Capture", ARPA-e IMPACCT Conference, Pittsburgh, PA, July 11, **2013**.
125. Eliseo Marin and Edward J. Maginn, "Moelcular Dynamics and Monte Carlo Simulation of Ionic Liquids", Annual AFOSR Contractors meeting, Edwards Air Force Base, CA, May 21, **2013**.
126. Surya Tiwari and Edward J. Maginn, "Stabilities of Actinyl Ion Complexes in Aqueous Phase" Joint Annual Meeting of the Geological Association of Canada and the Mineralogical Association of Canada, May 22, **2013**.
127. Edward Maginn, "Powering the Planet in a Carbon Constrained World", Hesburgh Lecture to the Silicon Valley Notre Dame Alumni Club Santa Clara, CA, Sept. 20, **2013**.
128. Surya Tiwari and Edward J. Maginn, "Stabilities of Actinyl Ion Complexes in Aqueous Phase", workshop on Materials Modeling and Simulation for Nuclear Fuels, Chicago, IL, Oct. 14, **2013**.

129. Katie Maerzke, William F. Schneider and Edward J. Maginn, "Uranyl(VI) and Plutonyl(VI) Coordination and Dynamics in a Task-Specific Ionic Liquid", workshop on Materials Modeling and Simulation for Nuclear Fuels, Chicago, IL, Oct. 14, **2013**.
130. Brian Yoo, Edward J. Maginn and Y. Elaine Zhu, "Interaction of Ionic Liquids with Lipid Biomembrane: Implication from Supramolecular Assembly to Cytotoxicity", AIChE Annual Meeting, San Francisco, CA, Nov. **2013**.
131. Akash Sharma, Edward J. Maginn and Mark J. McCready, "Experimental and Simulation Analysis of a Mixture of [C_6mim][NTf_2] and Tetraglyme", AIChE Annual Meeting, San Francisco, CA, Nov. **2013**.
132. Amir Vahid and Edward J. Maginn, "Molecular Modeling and SAFT Modeling of Solvation in Ionic Liquids", AIChE Annual Meeting, San Francisco, CA, Nov. **2013**.
133. Ramesh Singh and Edward J. Maginn, "The Solubility of Carbon Dioxide, Hydrogen and their Mixture in the Ionic Liquids 1-alkyl-3-methylimidazolium bis(trifluoromethanesulfonyl)amide ([C_6mim^+][Tf_2N^-])", AIChE Annual Meeting, San Francisco, CA, Nov. **2013**.
134. Edward Maginn, "Powering the Planet in a Carbon Constrained World", Hesburgh Lecture, Tri-State Notre Dame Club, Evansville, IN, Feb 22, **2014**.
135. Katie Maerzke, William Schneider and Edward J. Maginn, "Uranyl(VI) and Plutonyl(VI) Coordination and Dynamics in a Task Specific Ionic Liquid", American Chemical Society meeting, Dallas, TX March 18, **2014**.
136. Katie Maerzke, William Schneider and Edward J. Maginn, "Phase Equilibria and Thermophysical Properties of Ionic Liquid / Water Mixtures", American Chemical Society meeting, Dallas, TX, March 19, **2014.**
137. Daniela Kerlé and Edward J. Maginn, "Computational Study of Alcohols in Ionic Liquids", American Chemical Society meeting, San Francisco, CA, August 13, **2014**.
138. Yong Zhang and Edward J. Maginn, "Molecular Dynamics Studies of Dynamic Properties in Ionic Liquids", American Chemical Society meeting, San Francisco, CA, August 14, **2014**.
139. Eliseo Marin-Rimoldi and Edward J. Maginn, "Force Field Assessment for Predicting Vapor-Liquid Equilibrium of Water in Ionic Liquids", AIChE National Meeting, Atlanta, GA, Nov. 17, **2014**.
140. Jindal K. Shah, Eliseo Marin-Rimoldi and Edward J. Maginn, "Cassandra: A Novel, Open-Source Monte Carlo Molecular Modeling Platform for Materials Modeling", AIChE National Meeting, Atlanta, GA, Nov. 17, **2014**.
141. Yong Zhang and Edward Maginn, "Molecular Dynamics Studies of Viscosity in Branched / Linear Ionic Liquids", 6th International Congress on Ionic Liquids, Jeju, Korea, June 17, **2015**.
142. Daniela Kerlé, Bernd Rathke, Johannes Kiefer and Edward J. Maginn, "Solvation Behavior of Alcohols in Ionic Liquids", Foundations of Molecular Modeling and Simulation, Mt. Hood, OR, July 14, **2015**.
143. Eliseo Marin-Rimoldi, Jindal Shah and Edward Maginn, "Cassandra: A Monte Carlo Framework for Material Property Prediction", Foundations of Molecular Modeling and Simulation, Mt. Hood, OR, July 14, **2015**.
144. Daniela Kerlé, Bernd Rathke, Johannes Kiefer and Edward J. Maginn, "Solvation Behavior of Alcohols in Ionic Liquids", joint meeting of the European Molecular Liquids Group / Japanese Molecular Liquids Group, Rostock, Germany, Sept. 9, **2015**.

145. Edward Maginn, Flash Panel on Laudato Si, Kellogg Institute, University of Notre Dame, Oct. 14, **2015**.
146. Akihito Otani, Yong Zhang, Eiji Kamio, Hideto Matsuyama, and Edward J. Maginn, "Molecular Design of High CO_2-Reactivity and Low Viscosity Ionic Liquids for CO_2-Separative Facilitated Transport", AIChE Annual Meeting, Salt Lake City, UT, Nov. 11, **2015**.
147. Ryan Gotchy Mullen, Steven Corcelli, and Edward J. Maginn, "Molecular Simulation of CO_2 Absorption in the Ionic Liquid [P_{2228}^+][2CNpyr$^-$] Using Reaction Ensemble Monte Carlo", AIChE Annual Meeting, Salt Lake City, UT, Nov. 11, **2015.**
148. Edward Maginn, "Powering the Planet in a Carbon Constrained World", Hesburgh Lecture, Notre Dame Club of Northeast New York, Albany, NY, Dec. 11, **2015.**
149. Yushan Zhang, Yong Zhang, Mark J. McCready and Edward J. Maginn, "Membrane Separation of Biomolecules: A Coarse Grained Molecular Dynamics Study", Midwest Thermodynamics and Statistical Mechanics Conference, Miami University, Oxford, OK, May 25, **2016**.
150. Ken Newcomb and Edward J. Maginn, "A Molecular Dynamics Study of Actinide Nanoclusters", Midwest Thermodynamics and Statistical Mechanics Conference, Miami University, Oxford, OK, May 26, **2016**.
151. Ryan G. Mullen, Steve Corcelli and Edward J. Maginn, "Molecular Simulation of CO_2 Absorption in the Ionic Liquid [P2228][2-CNpyr] Using Reaction Ensemble Monte Carlo", Midwest Thermodynamics and Statistical Mechanics Conference, Miami University, Oxford, OK, May 27, **2016**.
152. Akash Sharma, Yong Zhang and Edward Maginn, "How Mixing Tetraglyme with Ionic Liquid Changes Volumetric and Transport Properties: An Experimental and Computational Study", 18th International Meeting on Lithium Batteries, Chicago, IL, June 19-24, **2016**.
153. Akash Sharma, Yong Zhang and Edward Maginn, "How Mixing Tetraglyme with Ionic Liquid Changes Volumetric and Transport Properties: An Experimental and Computational Study", Gordon Research Conference on Ionic Liquids, Newry, ME, August 17, **2016**.
154. Brian Yoo, Yingxi Zhu and Edward J. Maginn, Elucidating the Cytotoxic Interactions of Ionic Liquids Toward a Lipid Biomembrane", Gordon Research Conference on Ionic Liquids, Newry, ME, August 17, **2016**.
155. Ryan Gotchy Mullen, Steven Corcelli and Edward J. Maginn, "Molecular Simulation of CO2 Absorption in the Ionic Liquid [P2228][2-Cnpyr] Using Reaction Ensemble Monte Carlo", AIChE Annual Meeting, San Francisco, CA, Nov. 14, **2016.**
156. Brian Yoo, Yongxi Elaine Zhu and Edward J. Maginn, "Elucidating the Cytotoxic Mechanism of Imidazolium-Based Ionic Liquids Via Molecular Simulations", AIChE Annual Meeting, San Francisco, CA, Nov. 16, **2016**.
157. Eliseo Marin-Rimoldi and Edward J. Maginn, "Recent Advances in the Development of Cassandra: An Open Source Monte Carlo Framework for Phase Equilibria Calculations", AIChE Annual Meeting, San Francisco, CA, Nov. 14, **2016**.
158. R. Yang, K. Takechi, Y. Zhang and Edward J. Maginn, "Investigation of Solvation Structure and Battery Performance of Highly-Concentrated Aqueous Meo-TEMPO Catholyte", Electrochemical Society Meeting, National Harbor, MD, October 4, **2017**.
159. Yong Zhang, Kensuke Takechi, Ruidong Yang, and Edward Maginn, "Investigation of the Solvation State of Solvate Ionic Liquid: Li/TFSI/MT Mixtures with Water", International Conference on Ionic Liquid-Based Materials, Santiago de Compostela, October 24, **2017**.

160. Cassiano G. Aimoli, Danilo P. de Carvalho, Pedro A. P. Filho and Edward J. Maginn, "Thermodynamic Properties and Fluid Phase Equilibria of Natural Gas Containing CO_2 and H_2O at Extreme Pressures for Injection in the Brazilian Pre-salt Reservoirs", Offshore Technology Conference Brazil, Rio de Janeiro, Brazil, Oct. 24-26, **2017**.
161. Ken Newcomb and Edward J. Maginn, "A Molecular Dynamics Study of Actinide Nanoclusters", AIChE Annual Meeting, Minneapolis, MN, Oct. 30, **2017**.
162. Ryan Gotchy Mullen and Edward J. Maginn, "Reaction Ensemble Monte Carlo Simulations of Xylene Isomerization Under Confinement", AIChE Annual Meeting, Minneapolis, MN, Oct. 31, **2017**.
163. Michael Humbert, Yong Zhang and Edward J. Maginn, "Assessing the Reliability of Computing Ion Pair Lifetimes and Diffusivity to Predict Experimental Viscosity Trends of Ionic Liquids ", AIChE Annual Meeting, Minneapolis, MN, Nov. 1, **2017**.
164. Ryan Gotchy Mullen and Edward J. Maginn, "Reaction Ensemble Monte Carlo: Applications to Ionic Liquids", AIChE Annual Meeting, Minneapolis, MN, Nov. 2, **2017**.
165. Tuanan da Costa Lourenço, Yong Zhang, Luciano da Costa, and Edward Joseph Maginn, "A molecular dynamics study of lithium-containing aprotic heterocyclic ionic liquids", XVII Brazilian MRS meeting, Natal-RN, Brazil, Sept. 16, **2018**.

Grants and Contracts

1. "Advanced Molecular Simulations Applied to Zeolites" (PI), Dow Chemical Company, $35,750 (1/96-5/97).
2. "Laboratory for Distributed Computing and Visualization" (co-PI with M. Stadtherr, J. Westerink and A. Lumsdaine), Unit Specific Request Program, Notre Dame Office of Information Technology, $15,000, (4/97).
3. "Development and Utilization of Molecular Simulations in Engineering Education and Research" (PI), National Science Foundation Faculty Early Career Development (CAREER) Program, $300,000 (6/97-5/01).
4. "Molecular Simulation of Additive Performance in Boundary Lubrication" (PI), ALCOA Foundation, $10,000, (6/97-5/98).
5. "Molecular Dynamics Simulations of Macromolecules" (PI, with co-PI Davide Hill), National Center for Supercomputing, 20,000 service units, (12/01/97-11/30/98).
6. "Scalable Shared Memory: Case Studies" (co-PI with N. Chrisochoides, A. Lumsdaine, M. Stadtherr, R. Stevenson, J. Westerink, M. Lemmon, and P. Antsaklis), IBM Shared University Research Project, $309,544 in equipment and software, (5/98-4/99).
7. "Scalable Meta-Computing for Computational Science and Engineering", (co-PI with A. Lumsdaine, N. Chrisochoides, M. Stadtherr, R. Stevenson and J. Westerink), Department of Defense DURIP program, $250,000, (1/98-12/98).
8. "Molecular Simulation and Measurement of Adsorption and Diffusion in Microporous Materials" (PI), The BOC Group, $10,000, (5/98-4/99).
9. "Configurational-Bias Monte Carlo Simulation Methodology Development" (PI), Molecular Simulations Inc., $5,653 plus $49,100 in software (5/98-4/00).
10. "Molecular Dynamics Simulations of Complex Systems" (co-PI with H.-C. Chang), $20,000, Mobil Foundation, (4/98-3/00).
11. "WWW-Based Modules for Introduction of Molecular Simulation into the Chemical Engineering Curriculum" (co-PI with R. Rowley, D. Kofke, A. Panagiotopoulos, A. Chialvo,

R. Snurr, R. Terry, P. Cummings and P. Westmoreland), National Science Foundation Curriculum and Coarse Development Program, $332,800, (1/98-12/01).

12. "1998 Midwest Thermodynamics Conference" (co-PI with J. F. Brennecke), National Science Foundation, $4,936, (5/98-4/99.
13. "Design and Evaluation of Room Temperature Ionic Liquids for Green Chemical Processing" (co-PI with J. F. Brennecke, E. Beckman, K. Hutchenson and G. Proulx), National Science Foundation, $480,000, (6/00-5/03).
14. "Experimental and Molecular Modeling Investigations of Binary Adsorption in Zeolites and Functionalized Mesoporous Materials" (PI), The Petroleum Research Fund, $60,000, (9/1/00-8/31/02).
15. "Engineering Functionalized Mesoporous Materials for Selective Separations" (PI), National Science Foundation New Technology for the Environment program, $73,772, (9/1/00-8/31/02).
16. "Acquisition of a High-Performance Computing System" (co-PI with O. Wiest, D. Gezelter, M. Stadtherr, and A. Barabasi), National Science Foundation, $150,000, (9/1/00-8/31/01).
17. "Designing Nanostructured Catalysts to Exploit Mass Transfer Enhancement Caused by Macroscale Hydrodynamics" (co-PI with M. McCready), National Science Foundation, $99,854, (07/15/01-06/30/02).
18. "Strategic Design and Optimization of Inorganic Sorbents for Cesium, Strontium and Actinides" (co-PI with D. Hobbs, M. Nyman and A. Clearfield), Department of Energy, total project cost of $1,029,000, with $169,000 at Notre Dame, (9/15/01-9/14/04).
19. "Pyridinium-based Ionic Liquids: New Non-Volatile Solvents for Industrial Applications", (co-PI with J. Brennecke, M. Stadtherr, D. Lodge, C. Kulpa and G. Lamberti), Indiana 21st Century Research and Technology Fund, $1,363,099 (2/1/03-1/31/06).
20. "Determination of Physical Properties of Energetic Ionic Liquids Using Molecular Simulations" (PI), Air Force Office of Scientific Research, $242,466 (04/01/03 – 12/31/06).
21. "Simulation of Incoherent Inelastic Neutron Scattering Spectra of Ionic Liquids" (PI), Pittsburgh Supercomputer Center, 10,000 service units, (07/15/03-07/14/04).
22. "Design and Evaluation of Ionic Liquids as Novel CO_2 Absorbents", (PI, with co-PI J. Brennecke), Department of Energy", $404,106, (7/16/04-7/15/07).
23. "Strategic Design and Optimization of Inorganic Sorbents for Cesium, Strontium and Actinides" (co-PI with D. Hobbs, M. Nyman and A. Clearfield), Department of Energy, $1,199,000 ($184,000 at Notre Dame), (10/01/04 – 09/30/07).
24. "High Temperature Ionic Liquid Lubricant for Advanced Aircraft Turbine Engines" (PI, with co-PI J. Brennecke), Foster-Miller Inc. and Air Force Office of Scientific Research, $35,498, (Nov. 15, 2004-May 14, 2005).
25. "Ionic Liquids for Utilization of Waste Heat from Distributed Power Plants" (co-PI with J. Brennecke, S. Paolucci, M. Sen, and M. A. Stadtherr), Department of Energy, $1,546,498, (Aug 15, 2005-Aug 14, 2006).
26. "Mercury-Free Electrical Switch" (PI, with co-PI J. F. Brennecke), Infoscitex and Environmental Protection Agency, $18,000, (3/1/06-8/15/06).
27. "Ionic Liquids for Utilization of Waste Heat from Distributed Power Plants" (co-PI with J. Brennecke, S. Paolucci, M. Sen, and M. A. Stadtherr), Department of Energy, $1,350,000, (Aug 15, 2006-Aug 14, 2008).

28. “Ionic Liquids: Breakthrough Absorption Technology for Post-Combustion CO_2 Capture” (PI, with co-PI J. Brennecke and W. Schneider), Department of Energy, $3,008,451, (March 1, 2007-July 15, 2010).
29. “Determination of Physical Properties of Ionic Liquids Using Molecular Simulations”, (PI), Air Force Office of Scientific Research, $345,000, (Jan 1, 2007-May 31, 2010).
30. “GOALI - Atomistic Simulations of the Physical Properties and Phase Behavior of Ionic Liquid / Gas Mixtures”, (PI, with co-PI Mark Shiflett and A. Yokozeki), National Science Foundation, $109,321, (Aug 15, 2007-July 31, 2009).
31. “Technologies for Developing Predictive Atomistic and Coarse-Grained Force Fields for Ionic Liquid Property Prediction”, (co-PI with Marcus Martin (Useful Bias, Inc.), Mark Gordon (Iowa State), Robin Rogers (University of Alabama), and Greg Voth (University of Utah)), Air Force STTR Program, $17,500 to Notre Dame, (Oct. 1, 2007-Feb 29, 2008).
32. “Acquisition of a mid-range computational facility for design of new materials by multi-scale modeling”, (co-PI with Mark Gordon, Iowa State), Air Force DURIP program, $245,000 (Oct. 1, 2008-Sept 20, 2009).
33. “Notre Dame Geothermal Ionic Liquids Research” (co-PI with PI Joan Brennecke and co-PIs Mark McCready, Mark Stadtherr, Samuel Paolucci and Mihir Sen), Department of Energy, $984,000 (Aug. 1, 2008-July 31, 2010).
34. “Notre Dame Geothermal Ionic Liquids Research: Ionic Liquids for Utilization of Geothermal Energy”, (co-PI with PI Joan Brennecke and co-PIs Mark McCready, Mark Stadtherr, Samuel Paolucci and Mihir Sen), Department of Energy, $951,500 (Aug 1, 2010- July 31, 2012).
35. “Materials Science of Actinides”, (co-PI with Peter Burns, Jeremy Fein, Lynda Soderholm and PIs from the University of Michigan, University of California at Davis, Rensselaer Polytechnic University, and George Washington University), $21,689,042 (total award; ca. $500,000 to EJM), (July 1, 2009-June 30, 2014).
36. “Molecular Simulations in Support of Materials Science of Actinides”, National Energy Research Scientific Computing Center, 15,000 Cray XT4-equivalent MPP hours and 8,000 SRUs (Feb1, 2010 – Jan 31, 2011).
37. “Thermally-stable Ionic Liquid Carriers for Nanoparticle-based Advanced Heat Transfer in Concentrating Solar Energy Applications”, (co-PI with Elise Fox, Savannah River National Lab and Jamil Khan, University of South Carolina), Department of Energy, total award $1,005,000 ($295,167 to Notre Dame), February 1, 2010 – January 31, 2013).
38. “Molecular Simulation of Ionic Liquids: Physical Properties, Melting Points, and Mixing Behavior”, (PI), Air Force Office of Scientific Research, $350,272, (June 1, 2010-May 31, 2013).
39. “Molecular modeling and experimental investigation of the structure and dynamics of confined ionic liquids and their performance in gas separations” (PI, with S. Vasenkov, Univ. of Florida and co-PI J. Shah, Notre Dame), National Science Foundation, $247,300 (Notre Dame share), (July 1, 2010 – June 30, 2013).
40. “Phase Changing Ionic Liquids for CO_2 Capture”, (co-PI with J. Brennecke, W. Schneider, M. McCready and MATRIC), DOE ARPA-e, $2,559,563 ($228,158 to EJM) (July 1, 2010-June 30, 2013).
41. “Development of Materials for Improved Secondary Battery Technology”, (subcontract from Mississippi State University, co-PIs with J. Brennecke, P. McGinn, A. Seabaugh, S. Fullerton and P. Kamat), U.S. Army Tank Automotive Research, Development, and Engineering Center, $1,300,000, (May 15, 2010-May 14, 2012).

42. "Atomistic Simulation of Actinides", PI, National Energy Research Scientific Computing Center, Berkeley, CA, 58,000 Cray XT4-equivalent MPP hours, (Jan 1, 2011-Dec 31, 2011).
43. "Next Generation Ionic Liquids for Plutonium Science, Separation and Production", (co-PI with J. Brenncke and W. Schneider), subcontract from Los Alamos National Laboratory, $409,069, (October 1, 2010-September 30, 2013).
44. "Atomistic Simulation of Impurities in Metals", ExxonMobil, $15,000, (Nov. 1, 2008-Dec. 21, 2012).
45. "Compact Efficient Air Conditioning with Ionic Liquid Based Refrigerants", co-PI with PIs William Schneider, Mihir Sen, Joan Brennecke, Mark McCready and Mark Stadtherr), DOE ARPA-e, ($331,631 to EJM), (Sept 1, 2010-Aug 31, 2013).
46. "An Integrated Molecular Simulation, Biophysical Experimentation and Toxicology Bioassay Approach for Mechanistic Understanding of Toxic Effects of Ionic Liquids", NSF, $346,820, Co-PI; Lead PI: Jindal Shah; other Co-PIs Elaine Zhu and Gary Lamberti. (10/01/11 – 09/30/14).
47. "Chemically Complexing Ionic Liquids for Pre-Combustion CO_2 Capture", Global Climate and Energy Project, Stanford University, Co-PI; other PIs J. Brennecke, W. Schneider, B. Ashfeld, M. Stadtherr, $1,877,781, (Oct. 1, 2012 – September 30, 2015).
48. "PFI-BIC: Market-Guided Ionic Liquid Discovery and Design", PI, with co-PIs Joan Brennecke, Peter Kilpatrick, Mark McCready and William Schneider, $540,537, (Sept 1, 2012-Aug 31, 2015).
49. "Computational Tools in Support of the Electrolyte Genome: Joint Center for Energy Storage Research", PI, Lawrence Berkeley National Laboratory and Argonne National Laboratory, $566,731, Sept. 30, 2013-June. 30, 2018.
50. "SI2-SSE: Development of Cassandra, A General, Efficient and Parallel Monte Carlo Multiscale Modeling Software Platform for Materials Research", PI, with co-PI Jindal Shah, NSF, $395,133, Oct. 1, 2013-Sept. 30, 2018.
51. "Extraction of Natural Products", PI, University of Notre Dame and Pontifical University of Chile, $29,500, July 1, 2014-June 30, 2017.
52. "Materials Science of Actinides", (Peter Burns PI), University of Notre Dame and various other universities, $10,400,000 (ca. $175,000 to EJM), August 1, 2014-July 31, 2018.
53. "Synthesis, Characterization and Simulations of Ionic Liquids", Air Force Office of Scientific Research, PI, $339,903, Sept 1, 2014-Aug. 31, 2017.
54. "Rapid Calculation of Isotherms for Absorption of Gases into Reactive Ionic Liquids", Notre Dame Strategic Research Investment, co-PI with Steve Corcelli, $75,000, July 1, 2014-June 30, 2016.
55. "Collaborative Research: Describing Macromolecular Transport through Chemically-tuned Nanoporous Membranes via Theory, Computation, and Experiment", co-PI with William Phillip, NSF, $150,145, July 1, 2015-June 30, 2018.
56. "Investigation of the solvation state of 4-methoxy-2,2,6,6-tetramethylpiperidine 1-oxyl / lithium bis(trifluoromethanesulfonyl)imide mixtures with water", PI, Toyota Motor Engineering Manufacturing North America, Inc., $86,942, April 14, 2016-March 31, 2018.
57. "Combined Quantum-Classical Theoretical Studies of Processes in the Condensed Phase", PI, Air Force Office of Scientific Research, $398,671, 05/01/2018-04/30/2021.
58. "Collaborative Research: NSCI Framework: Software for Building a Community-Based Molecular Modeling Capability Around the Molecular Simulation Design Framework (MoSDeF)", PI, National Science Foundation, $638,861, 10/01/2018-09/30/2022.

59. "Joint Center for Energy Storage Research 2.0", PI, Department of Energy, subcontract from Argonne National Lab, $403,246, 07/01/2018-06/30/2023.
60. "Breakthrough Electrolytes for Energy Storage (BEES)", PI, Department of Energy, subcontract from Case Western Reserve University, $573,552, 08/01/2018-07/31/2022.
61. "Molten Salts in Extreme Environments", PI, Department of Energy, subcontract from Brookhaven National Lab, $769,680, 08/01/2018-07/31/2022.

Doctoral Dissertations Directed (current position)

1. Yiannis Kaznessis (joint with D. A. Hill), "Molecular Dynamics Simulations of Macromolecules. Comparison with Dielectric Spectroscopy Experiments", (**1999**). (University of Minnesota)
2. Michael Macedonia "Development and Application of Advanced Monte Carlo Techniques for the Study of Adsorption Related Processes in Zeolites", (**2000**). (CEO, Veracity Forecasting, Pittsburgh, PA)
3. Loukas Kioupis "Molecular Simulations of Hydrocarbon Lubricants: Impact of Molecular Architecture on Performance Properties", (**2000**). (General State Chemical Laboratories of Greece)
4. Gaurav Arya (joint with H. –C. Chang) "Molecular Simulation of Transport in Nanoporous Materials", (**2003**). (Duke University)
5. Jennifer Anthony (joint with J. F. Brennecke), "Gas Solubility ion Ionic Liquids", (**2004**). (Kansas State University)
6. Jindal Shah, "Monte Carlo Simulations of the Ionic Liquid 1-butyl-3-methylimidazolium hexafluorophosphate", (**2004**). (Oklahoma State University)
7. Jacob Crosthwaite (joint with J. F. Brennecke), "Ionic Liquid Phase Equilibria Measurements", (**2005**). (Dow Chemical)
8. Timothy I. Morrow (joint with J.F. Brennecke), "Development and Application of Molecular Dynamics Methods to the Study of Ionic Liquids", (**2005**). (ExxonMobil)
9. James Larentzos, "Molecular Modeling of Cation and Water Adsorption in Crystalline Titanosilicate and Polyoxoniobate Materials", (**2006**). (U. S. Army Research Laboratory).
10. David Eike, (joint with J. F. Brennecke), "Development and Application of Molecular Simulation Methods for Prediction of Melting Points", (**2006**). (Procter and Gamble)
11. Cesar Cadena, "Molecular Simulation of Energetic Ionic Liquids", (**2006**). (Easy Motto Corp.)
12. Manish Kelkar, "Computing Transport Properties of Molecular and Ionic Fluids using Atomistic Simulations", (**2007).** (AbbVie)
13. Brian R. Novak (joint with M. J. McCready), "Molecular Simulation Studies of Heterogeneous Bubble Nucleation: Effects of Surface Chemistry and Topology", (**2007).** (Louisiana State University)
14. Saivenkataraman Jayaraman, "Computing Thermodynamic and Transport Properties of Room Temperature Ionic Liquids and Molten Salts from Atomistic Simulations", (**2009**). (Chemours)
15. Craig Powers, "Monte Carlo Simulation of Adsorption and Ion Exchange in Nanoporous Materials", (**2011**). (Aspen Technology)
16. Andrew Paluch, "Efficiently Modeling the Solution Phase Behavior of Soluble Solid Solutes Via Molecular Simulation and Solution Theory", (**2013**) (Miami University, OH).

17. Marcos Perez-Blanco, "Atomistic Simulation of Ionic Liquid Interfaces", (**2013**) (Ingersoll-Rand).
18. Hao Wu, "Dynamics and Water Solubility of Ionic Liquids for CO_2 Capture Using Molecular Dynamics Simulation", (**2013**).
19. Akash Sharma (joint with M. McCready) "Simulations and Experiments of Interfacial Mass Transfer in Ionic Liquids", 2011-2013. (Deceased, posthumous PhD awarded **2015**).
20. Surya Tiwari, "Thermodynamics and Speciation of Actinide Materials in the Condensed Phase Using Atomistic Simulations", (**2015**) (National Energy Technology Laboratory).
21. Samir Budhathoki, "Molecular Modeling and Simulation Study of the Structure and Dynamics of Confined Ionic Liquids and Their Performance in Gas Separations", (**2015**), (National Energy Technology Laboratory).
22. Eliseo Marin Rimoldi, "Monte Carlo Simulations of Phase Equilibria and Software Development", (**2017**) (Virginia Tech).
23. Brian Yoo (joint with Y. Zhu), "Molecular Simulation of Surfactant Interfaces", (**2017**) (BASF).
24. Quintin Sheridan (joint with W. Schneider), "Simulation Study of CO_2-Reactive Aprotic Heterocyclic Anion Ionic Liquids: Water Interactions, Liquid Structure and CO_2 Solubility", (**2017**). (Sales Partnerships Inc.)

Doctoral Dissertations under Direction

1. Ken Newcomb, "Molecular Modeling of Actinide Clusters in Solution", 2014-present.
2. Michael Humbert, "Rapid Screening of Electrolytes via a Materials Genome Approach", 2014-present.
3. Yushan Zhang, "Fundamental Studies of Liquid Dynamics via Molecular Dynamics", 2014-present.
4. Jacob Gerace, "Modeling Liquid-Liquid Equilibria Using Advanced Monte Carlo Methods", 2016-present.
5. Haimeng Wang, "Molecular Simulation of Molten Salts for Nuclear Energy Applications", 2017-present.
6. Garrett Tow, "Rare Event Modeling of Solid Composite Propellant Aging", 2017-present.
7. Derrick Poe, "Molecular Modeling of Deep Eutectic Solvents for Flow Batteries", 2018-present.
8. Bridgette Befort, "Molecular Design and Optimization for Advanced Separation Processes", 2018-present.

Masters Dissertations Directed

1. Darrin Moore, "Experimental Studies of Gas Adsorption on Microporous Materials", (2000). (Dupont Nutrition and Health)
2. Jing Chen (joint with A. Varma), "Experimental and Computational Studies of Zeolite Membranes", (2000). (Diagnostic Products Corp.)
3. Robbie Landis, "Synthesis and Characterization of Functionalized Mesoporous Silica for the Remediation of Heavy Metals from Aqueous Solution", (2002). (Y-12 National Security Complex)
4. Pavithra Tiruppathi, "Molecular Dynamics Simulations of Ionic Liquid Nanodroplets in Electric Fields", (2011) (Syntellect).

Postdoctoral Researchers Under Direction
None

Postdoctoral Researchers Directed (current position)

1. Robert Nooney, "Synthesis of Functionalized Mesoporous Materials", 1999-2001. (Dublin City University)
2. Qing Dai, "Encapsulated Homogeneous Catalysts" (with A. Ostafin, S. Brown and D. Meisel), 2001-2002. (Monash University)
3. Haizhong Zhang, "Molecular Modeling of Gas Solubility in Ionic Liquids", 2004-2006. (Fisher-Klosterman)
4. Wei Shi, "Molecular Modeling of Ion Exchange and Ionic Liquid Properties", 2006-2008. (National Energy Technology Laboratory)
5. Keith Gutkowski, "Force Field Development for Ionic Liquids", 2007-2008. (BASF)
6. Manish Kelkar, "Experiments and Atomistic Simulation of Hydrofluorocarbon Solubility in Ionic Liquids", 2007-2008. (AbbVie)
7. Tom Rosch, "Development of Reactive Monte Carlo Methods for CO_2 Capture", 2008-2011. (National Institute of Standards and Technology)
8. Craig Tenney, "Molecular Simulation of the Thermodynamic and Transport Properties of Ionic Liquid Heat Transfer Fluids", 2008-2011 (Sandia National Laboratory)
9. Hongjun Liu, "Molecular Simulation of Polyelectrolytes in Electric Fields", 2009-2012. (Oak Ridge National Laboratory).
10. Neeraj Rai, "Molecular Simulations of Actinides and Ionic Liquids", 2009-2012 (Mississippi State University).
11. Vladimir Pomogaev (co-advised with W. Schneider), "Computational Studies of Actinides", 2011-2012. (Tomsk State University).
12. Amir Vahid, "Thermal Properties of Ionic Liquids from Molecular Simulations", 2012-2013. (Life Elixir, LLC).
13. Yong Zhang, Simulations of Solid-Liquid Phase Equilibria in Ionic Liquids", 2011-2013. (Notre Dame)
14. Ramesh Singh, "Molecular Simulation of Pre-Combustion Gas Solubility in Ionic Liquids", 2012-2014. (Univ. Pittsburgh, Johnstown).
15. Sandip Khan, "Modeling Actinide Solid Solutions", 2012-2014. (Department of Chemical Engineering, Indian Institute of Technology, Patna).
16. Katie Maertzke, "Molecular Modeling of Actinide / Ionic Liquid Systems", 2012 – 2014. (Los Alamos National Laboratory).
17. Jindal Shah, "Development of Cassandra, and Open Source Monte Carlo Code", 2007-2014 (Department of Chemical Engineering, Oklahoma State University).
18. Daniela Kerlé, "Computing Liquid-Liquid Equilibria of Alcohols and Ionic Liquids", 2013-2015. (University of Bremen, Germany).
19. Ryan Mullen, "Reactive Monte Carlo Method Development", 2015-2017. (Lawrence Livermore National Lab).

Research Professors / Staff Scientists Under Direction

1. Yong Zhang, 2013-present

Research Visitors

1. Dr. Gabrielle Raabe (Germany), 2009-2010
2. Prof. Lucienne Rominello (Brazil), 2012; 2014-2015
3. Prof. Luciano Costa (Brazil), 2012
4. Cassiano Aimoli (Brazil), 2012-2014
5. Marta Batista (Portugal), 2013
6. Luis Franco (Brazil), 2013-2014
7. Akihiro Otani (Japan), 2014-2015
8. Andreas Bröhl (Germany), 2015.
9. Nathalia Salles Vernin Barbosa (Brazil), 2015-2017.
10. Tuanan Cost Lorenço (Brazil), 2016-2017.
11. Dr. Jingqui Wang (China) 2017-2018.

Undergraduate Researchers under Direction

1. Olivia Garcia-Velez, "Monte Carlo Simulations of Liquids" (8/18-present).
2. Leah Fast, "Molecular Modeling of Imidazole" (8/18-present).

Undergraduate Researchers Directed

1. Ron Runnebaum, "Evidence for Resonant Diffusion Effects in Zeolites from Molecular Dynamics Simulations", (11/95-6/96).
2. Matt Macura, "Molecular Dynamics Simulations of Hydrocarbons in MCM-41", (12/96-5/97).
3. Renee Sehee, "Adsorption Measurements for Liquid Mixtures on Zeolites", (6/97-5/98).
4. James Kelly, "Adsorption of Organic Contaminants", (6/98-5/99).
5. Vincent Keating, "Excess Adsorption Measurements from Organic Liquid Mixtures", (5/99-5/00).
6. Christopher O'Keeffe, "Gibbs Ensemble Simulation of Hydrofluorocarbon VLE", (9/02-5/04).
7. Mary Ann Jentz, "Grand Canonical Monte Carlo Simulation of Adsorption in Nanoporous Materials", (8/04-5/05).
8. David Couling, "Quantitative Structure-Property Modeling of Ionic Liquid Toxicity and Thermal Stability", (8/04-5/06).
9. David Tagler, "Quantitative Structure-Property Modeling of Ionic Liquid Viscosity", (8/05-5/06).
10. Neil Reese, "Molecular Modeling of Cavitation", (8/05-5/06).
11. Nate Stober, "Atomistic Simulation of Ionic Liquid / Organic Species Mixtures", (9/06-5/07).
12. Tom Mazzacavallo, "Development of a force field database", (5/08-8/08).
13. Bryce Chung, "Development of a force field database", (5/08-5/10).
14. Patrick Yee, "Microscopic State of Ionic Liquid Ion Pairs At Low Concentrations In Water As Studied From Molecular Dynamics Simulations", (8/09-5/11).
15. Daniel Cryan, "Simulations of Aqueous System Transfer Free Energies", (4/10-9/10).
16. Cameron Vitter, "Expanded Ensemble Monte Carlo Simulations", (1/11-5/12).
17. David Smith, "Potential of Mean Force Calculations of Hydrated Ionic Liquid APIs", (1/12-5/13).

18. Rose Doerfler, "Simulating Ionic Liquids with Branched Alkyl Sidechains", (1/14-5/14).
19. Patrick Griffin, "Evaluating the Performance of the Cassandra Monte Carlo Package" (6/14-8/14).
20. Chris Dearolf, "Molecular Modeling of Ionic Liquids + Tetraglyme", (1/14-5/15).
21. Chris Gerik, "Computing the Viscosity of Polyether Molecules", (1/14-5/15).
22. Ian Tembe, "System Size Effects on Calculated Transport Properties", (8/15-12/15)
23. Edward Smierciak, "Simulating Water at an Ionic Liquid Interface", (8/15-5/16)
24. Greg Conti, "QSPR Modeling of Phase Change Materials", (1/16-5/16).
25. Gabrielle Dohman, "Simulating Phase Equilibria of Glymes", (3/16-5/16).
26. Brian Keene, "Developing Computational Resources for Cassandra", (8/14-5/16).
27. Sheridan Foy, "Gibbs Ensemble Phase Equilibria Simulations of Noble Gases in Ionic Liquids Using a Mie Potential", (1/16-5/18).
28. Matthew Howenstein, "Development of a Test Suite and Validation Studies for Cassandra", (9/16-5/18).
29. Mary McKinley, "Monte Carlo Simulations of Vapor-Liquid Equilibria", (1/18-5/18).

Other Notable Contributions

Educational Activities

- Developed Joule-Thomson educational module as part of the CACHE Molecular Modeling Task Force

- Workshop on Monte Carlo simulations, School of Advanced Studies In Applied Thermodynamics, Rio De Janeiro, Brazil, August, 2011.

- Workshop on molecular dynamics simulations, School of Advanced Studies In Applied Thermodynamics, Rio De Janeiro, Brazil, July, 2010, 2011.

- Workshop on Cassandra software and Monte Carlo methods, Pontificia Universidad Católica de Chile, Santiago, Chile, Jan. 2016; University of Notre Dame, June 5-10, 2016.

- Workshop on Cassandra software: Edward J. Maginn, Ryan Gotchy Mullen, Jindal K. Shah and Eliseo Marin-Rimoldi, "How to Use the Atomistic Monte Carlo Simulation Package Cassandra: Liquid Phase Properties and Vapor-Liquid Equilibria", AIChE Annual Meeting, Minneapolis, MN Oct. 29, 2017.

Consulting Work / Industrial Activities

- Scientific Advisory Team, Scienomics (2016-present)
- ExxonMobil EMRE (2014-present)
- Buckingham, Doolittle and Burroughs, LLP; expert witness on case involving zeolites (2007)
- Infoscitex (2006)
- Air Liquide (2006)
- Foster Miller (2005).

- The BOC Group, Murray Hill, NJ (1998 - 2000)
- Scientific advisor to the Catalysis and Sorption Consortium, Molecular Simulation Inc. This Consortium is comprised of roughly thirty companies in the petroleum, chemical and pharmaceutical industries, plus National Labs and various universities (1996-1997)

Technology Transfer Activities

- Co-founder of *Ionic Liquid Research Technologies, LLC*, a startup company in Notre Dame's Innovation Park (2011-2014).
- Developed *Flexisorb* molecular modeling program. This program is an implementation of a configurational-bias grand canonical Monte Carlo method developed as part of Michael Macedonia's PhD thesis. The program is available free of charge to academic users and has been incorporated into Molecular Simulation Inc.'s Cerius^2 commercial molecular modeling package. Cerius^2 is used by many of the top 50 chemical and petroleum companies.

Session Chair / Organizer for the following technical sessions / symposia:

- Department Heads Forum, AIChE Annual meeting, **2017**, **2018**.
- Co-organizer, "George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Alexis T. Bell", American Chemical Society meeting, New Orleans, LA, April 7-8, **2013**.
- Co-organizer, "Symposium in Honor of Alexis Bell's 70th Birthday", AIChE Annual Meeting, Pittsburgh, PA, Oct. 30-31, **2012**.
- Co-Organizer, "Ionic Liquid Modeling", International Conference on Chemical Thermodynamics, Buzios, Brazil, August **2012**.
- Co-Organizer "Ionic Liquids: Science and Applications", American Chemical Society National Meeting, and chair of Modeling, Simulation and Theory session, San Diego, CA March **2012**.
- Chair, Symposium on Ionic Liquids in Sustainable Energy and Fuels, ACS Meeting, Boston, MA, August **2010**.
- 8th World Congress on Chemical Engineering, Montreal, Quebec, Canada, August **2009**.
- Organizer, Symposium on Molecular Modeling of Ionic Liquids, American Chemical Society National Meeting, Philadelphia, PA, August, **2008**.
- Structure of Ionic Liquids session, 2nd International Congress on Ionic Liquids, Yokohama, Japan, August, **2007**.
- Symposium on Molecular Modeling of Ionic Liquids, ACS national meeting, San Francisco, CA, September, **2006**.
- Modeling Ionic Liquids Symposium coordinator, ACS Meeting Spring **2006**.
- Teaching Thermodynamics and Statistical Mechanics at the Graduate Level, **2004** AIChE Meeting.
- Advanced Fluids, AIChE Meeting ***2007-2009***.
- Transport in Nanostructured Porous Materials, AIChE Meeting **2004**.
- Ionic Liquids: Thermodynamic and Transport Properties, AIChE Meetings **2004-2006**.
- Nonequilibrium Molecular Dynamics, 15th Symposium on Thermophysical Properties,

June, **2003**.

- Advances in Simulation Techniques, Fundamentals of Molecular Modeling and Simulation, July, **2003**.
- Microscopic Modeling of Transport Processes, AIChE Meeting **2000, 2001 and 2003.**
- Thermodynamic Properties of Polymers II, AIChE Meeting **2002**.
- Young Faculty Forum AIChE Meeting **1999 and 2000**.
- General Papers on Thermodynamics and Transport Properties: Poster Session, AIChE Meeting **1999**.
- Thermodynamic Properties and Phase Behavior: General Papers, AIChE Meeting **1998**.

Professional Activities

- External Advisory Board, Department of Chemical and Biomolecular Engineering, Case Western Reserve University, **2017-present**.
- Editorial Advisory Board Member, *Journal of Chemical and Engineering Data*, **2016-present**.
- External Advisory Board, School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, **2014-2016**.
- Co-organizer, 2nd International Conference on Ionic Liquids in Separation and Purification Technology, Toronto, Canada, June 29-July 2, **2014**.
- International Committee for the XIX International Conference on Chemical Thermodynamics in Russia RCCT-2013, Samara, Russia, June 24-28, **2013**.
- Member, International Scientific Advisory Board, 5th Congress on Ionic Liquids, Algarve, Portugal, April 21-25, **2013**.
- Editorial Advisory Board of the *Journal of Physical Chemistry*, **2013-2015**.
- Conference Chair, Foundations of Molecular Modeling and Simulation international conference, July **2012**.
- Host Committee, 4th Congress on Ionic Liquids, Washington, D. C. June 15-18, **2011**.
- Member of Organizing Committee, Institute of Pure and Applied Mathematics workshop on Physical Frameworks for Sampling Chemical Compound Space, UCLA, May 16-20, **2011**
- Organizer, Midwest Thermodynamics and Statistical Mechanics Conference, University of Notre Dame, June 2-3, **2010**.
- Member of Scientific Committee, 8th World Congress of Chemical Engineering Symposium on Separation Science and Technology (**2009**).
- Trustee, Computer Aids for Chemical Engineering Education (CAChE) Corporation, **2009-present**.
- Elected Liaison Director, Computational Molecular Science and Engineering Forum, AIChE (**2007-2009**)
- Proposal Review Committee, Oak Ridge National Laboratory Center for Nanophase Materials Sciences (**2006-present**)
- Member of Editorial Board, *Fluid Phase Equilibria* (**2005-present**).
- Member, Scientific Advisory Committee, 8th International Conference on Fundamentals of Adsorption, Sedona, AZ, May, **2004**.
- Technical Participant, National Research Council's Workshop on Novel Approaches to Carbon Management, Irvine, CA Feb. **2003**.
- Participant, NIST workshop on future directions for molecular modeling (**2001**).

- Programming Chair, Area 1a (Engineering Sciences & Fundamentals: Thermodynamics and Transport Properties), Fall **1999** AIChE Meeting.
- Co-organizer, Midwest Conference on Thermodynamics and Statistical Mechanics (**1998**).
- Member, AIChE Area 1a Programming Committee (**1997-2003**).
- Participant, NSF workshop on "Future Directions in Molecular Simulations and Computational Chemistry: Fundamentals and Applications", (Nov. **1997**).
- Member, CAChE Corporation Task Force on Molecular Modeling (**1996-present**).

Service Activities at Notre Dame

- Appointed member, *ad hoc* committee on Notre Dame's Research Vision, **2018-present**.
- Appointed member, Decennial Academic Article Review Committee, **2017**.
- Endowed Chair appointment committee, **2016, 2017.**
- Dean's Appointee and Chair, Aerospace and Mechanical Engineering Department Chair Search Committee, **2016**.
- Appointed Chair, Advanced Studies Committee of the Academic Council, **2016-2017**.
- Department Chairs Advisory Group to the Provost, **2015-2017;** Chair, **2016-2017**.
- Elected member of the Executive Committee of the Academic Council, **2015-2017.**
- Appointed member, Academic Council, **2015-2018.**
- Member, Catholic Mission Focus Group, Core Curriculum Review Committee, **2015-2016**.
- Member, College of Engineering Elections Committee, **2013-2015**.
- Department Chair, Chemical and Biomolecular Engineering, **July 1, 2012-present**.
- Chair of *ad hoc* committee on Future and Role of Professional Science Master's Programs at Notre Dame, **2012**.
- Assessment Liaison for the Graduate School on the University Student Learning Outcomes Committee, **2011-2012**.
- Member of Valedictorian Section Committee, University of Notre Dame, **2010**.
- Associate Dean for Academic Programs, Notre Dame Graduate School, **2009-2012**.
- University Committee on Academic Technologies **2008-2009**.
- Provost's *ad hoc* committee on hiring Catholic faculty **2007**.
- Search Committee Member, Dean of the College of Engineering **2006-2007**.
- Search Committee Member, Director of Center for Research Computing **2006-2009**.
- Engineering College Council, **2005-2007**.
- Member of Center for Research Computing advisory committee **2005-2007**.
- Member, *ad hoc* Committee on Development of Courses at the Intersection of Science, Engineering, Technology and Society, College of Engineering **2004-2006**.
- Member, Engineering Advisory Committee on EG111/112 **2004-2006**.
- Graduate School Task Force on Financial Aid / Advancing Doctoral Education **2004**.
- Graduate Council Task Force on graduate student health insurance **2003-2004**.
- Elected College of Engineering representative Notre Dame Graduate Council **2003-2006**.
- Appointed member of Notre Dame Graduate Council **2002-2003**.
- Interdisciplinary Research Group Leader (Nanostructured Materials), Center for Molecularly Engineered Materials **2001-2006**.
- Director of Graduate Recruiting, Chemical and Biomolecular Engineering **2000-2002, 2004-2007, 2009**.

- Member, *ad hoc* committee on Information Technology in Engineering **1998-1999**.
- Chemical Engineering Graduate Recruiting Committee **1997, 1999**.
- Advisor to the Notre Dame AIChE Student Chapter **1996-2000**.
- Member, Engineering College Computing Committee **1996-2007**.

Agency Review Acitivities
- National Science Foundation
- ACS PRF
- NIH Modeling and Analysis of Biological Systems study section
- Air Force Office of Scientific Research
- DOE (BES, NETL)
- DOE Center for Nanophase Materials Sciences
- Qatar Foundation
- Argonne National Laboratory Center for Nanophase Materials

Journal Review Activities
- Accounts of Chemical Research
- Adsorption
- American Institute of Chemical Engineers Journal
- Angewandte Chemie International Edition
- Chemical Communications
- Chemical Engineering Science
- Chemical Physics Letters
- Chemical Reviews
- Crystal Growth and Design
- Fluid Phase Equilibria
- Industrial and Engineering Chemistry Research
- Journal of Chemical and Engineering Data
- Journal of Chemical Physics
- Journal of Chemical Theory and Computation
- Journal of Computational Chemistry
- Journal of Hazardous Materials
- Journal of Molecular Structure: THEOCHEM
- Journal of Physical Chemistry (A, B, C and Letters)
- Journal of the American Chemical Society
- Langmuir
- Macromolecules
- Microporous and Mesoporous Materials
- Molecular Physics
- Molecular Simulation
- Oil and Gas Science and Technology
- Physical Chemistry Chemical Physics
- Physical Review
- Physical Review Letters
- Polymer
- Proceedings of the National Academy of Science

- Science
- Thermochimica Acta