Chemically-Complexing Ionic Liquids for Pre-Combustion CO_2 Capture

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All researchers were at the University of Notre Dame. Please note that the post-doctoral and graduate student researchers held anywhere from 0-100% appointments on the GCEP project. Everyone is listed who contributed something to the project.

Abstract

In this project we used a systematic approach to the design and development of novel, chemically-complexing ionic liquids (ILs) for the separation of CO_2 from pre-combustion gases, as occur for example, in an integrated gasification combined cycle (IGCC) process for power generation. We investigated three new types of ILs for pre-combustion CO_2 capture: 1. Weak specific binding aprotic heterocyclic anionic (AHA) ILs; 2. ILs featuring

structural cooperative complexation; and 3. ILs featuring physical cooperative complexation.

Introduction

ILs are salts with low melting points, wide liquid phase operating ranges, and endless tunability. They are attractive for CO_2 capture because they can be used in conventional absorber/stripper equipment, their interactions with CO_2 and selectivity for absorption of CO_2 over other gases can be tuned exquisitely, they require no added water to serve as a diluent or carrier (which adds an energy penalty during regeneration for alkanolamine-based CO_2 capture), and they have the potential to operate at higher temperatures than traditional CO_2 absorption media.

Over the twelve years prior to this GCEP project, the IL research team at Notre Dame had made both fundamental scientific and technological advancements in the development of ILs for post-combustion CO_2 capture. We were the first to report high physical CO_2 solubility in ILs and have subsequently used a combination of theory, molecular simulation, and synthesis and testing of new materials, to develop ILs with even higher physical dissolution of CO_2 and high selectivity for CO_2 over O_2, N_2, H_2, CH_4, H_2S and other gases. Our funding from DOE NETL (since 2004) for post-combustion flue gas separations has led us to incorporate opportunities for chemical complexation with CO_2 in the ILs. Major advances have included doubling the capacity to 1 mole of CO_2 per mole of IL by incorporating the amine functionality on the anion, developing aprotic heterocyclic anions that completely eliminate the horrendous (i.e., orders of magnitude) increase in viscosity experienced by other ILs when they react with CO_2, and the ability to tune the reaction enthalpy. The purpose of the GCEP project was to further improve ionic liquids for CO_2 capture applications, including pre-combustion capture.

Background

During the course of this project, a number of papers appeared that contained data on the physical solubility of gases of interest in ILs. These included physical H_2S solubility in various ILs.[1-3] There were also publications of MD calculations of gas solubilities, including those of CO_2, H_2S and H_2, primarily in conventional ILs.[4,5] Three articles appeared reporting on efforts to increase CO_2 uptake by ILs to greater than 1 mole of CO_2 per mole of IL.[6-8] Luo et al. studied some hydroxypyridine-based ILs where they propose CO_2 addition to the oxygen, which then facilitates addition of CO_2 to the nitrogen of the pyridine ring.[6] The same group reported somewhat greater than 1/1 uptake for a carboxyl functionalized imidazolide.[7] Both of these studies use tetra-alkylphosphonium cations so CO_2 reaction with the phosphonium ylide (as explained in our previous annual report and below) may be contributing to the uptake. Note that this same group reported the reaction of CO_2 with phenolate anions.[9] We believe that they have misunderstood the mechanism of the CO_2 uptake. The third article does not suggest cooperativity, but demonstrates > 1/1 uptake for tetra-alkylammonium amino acid based ILs.[8] Recent work on H_2S solubilities has attempted the molecular simulation and modeling of the limited experimental data that is available.[10,11]

Results

In the first year of the project we made significant progress on the second class of compounds – ILs featuring structural cooperativity. This included quantum calculations

of binding energies of candidate materials, synthesis of three specific ILs designed for structural cooperativity in the complexation of CO_2, characterization of and measurement of the CO_2 capacity of these materials, and the development of a thermodynamic model for multi-site cooperative binding. In addition, we developed a method to predict the physical solubility of CO_2 and H_2 in ionic liquids, which is applicable for the use of all three types of IL materials in the separation of CO_2 from pre-combustion gases. Finally, we have discovered and fully characterized additional chemistry that is occurring when sufficiently basic anions are paired with phosphonium cations, which results in CO_2 complexation with the cation.

In the second year of the project, thermodynamic and process modeling clearly identified the ideal reaction enthalpies needed for an IL that exhibits cooperative binding in order to minimize the energy needed for a pre-combustion gas separation process. In addition, numerous compounds were synthesized, which were designed, based on quantum mechanics and molecular simulations, to exhibit structural cooperative CO_2 complexation for super-stoichiometric carbon capture. One of those compounds showed CO_2 uptake significantly greater than 1 mole of CO_2 per mole of IL. Significant progress was made in developing computational methods needed to explain physical cooperativity and we clearly demonstrated that water can be used to control CO_2 uptake through physical cooperativity. We experimentally measured both H_2S and N_2 solubilities in ILs and developed a method to rapidly predict physically dissolved mixed gas solubilities. We fully characterized a new route for CO_2 capture – by reaction of CO_2 with a phosphonium ylide.

In the final year of the project, thermodynamic and process modeling clearly identified the ideal reaction enthalpies needed for an IL that exhibits cooperative binding in order to minimize the *cost* needed for a pre-combustion gas separation process (previous work had focused just on *energy* use). Quantum chemical methods were used to predict β-enaminoimine-based anion structures that show promise for cooperative CO_2-binding. Some of these were synthesized, along with ILs based on bispyrroles, α-*N*-heterocyclic β-amino alcohols, *ortho*-amino phenol, and *N*-heteroaromatic-substituted proline derivatives. Only a few of the bispyrrole ILs, which do not have attractive physical properties, showed super-stoichiometric CO_2 uptake. The fundamental chemistry leading to these observations were explored both computationally and experimentally. We successfully showed how physical cooperativity can enhance CO_2 uptake, both through the effect of water and the development of a new route for CO_2 capture by ILs – by reaction of CO_2 with a phosphonium ylide. We measured the solubility of other gases present in pre-combustion and post-combustion flue gas in the ionic liquids, most notably, H_2S, which has high physical solubility. Finally, we developed a new method to calculate the uptake of CO_2 by reactive ionic liquids using molecular simulations and theory.

More details on these results can be found in the 2013, 2014 and 2015 Progress Reports, as well as the publications and presentations listed below.

Conclusions

In this project, we developed new ionic liquids that showed cooperativity and CO_2 uptakes well above 1 mole CO_2/mole IL. However, their physical properties are not attractive for industrial applications. We have also shown how physical cooperativity can be used to enhance CO_2 uptake and now better understand the CO_2 uptake chemistry. We have measured the physical solubility of gases of other gases of interest, including H_2S, O_2

and N_2. New molecular modeling and simulation methods were developed and used to design the new ILs and predict gas solubilities. Process modeling was used to identify the optimal physical and chemical properties. High viscosity and, subsequently, poor mass transfer, remains a challenge for using the ILs developed for practical CO_2 capture applications. Subsequently, two of the GCEP PIs, Profs. Joan Brennecke and Mark Stadtherr, have been awarded a three year project from the Department of Energy National Energy Technology Laboratory, to work with researchers at Lawrence Livermore National Laboratory to encapsulate ILs in polymeric microspheres. By massively increasing the surface area, the mass transfer challenges associated with the ILs can be met.

Publications and Presentations

Publications

1. Monika Vogt, Joshua E. Bennett, Yong Huang, Chao Wu, William F. Schneider, Joan F. Brennecke and Brandon L. Ashfeld, "Solid State Covalent Capture of CO_2 Using *N*-Heterocyclic Carbenes," Chemistry – A European Journal, 2013, 19(34), 11134-11138.
2. Thomas R. Gohndrone, Tae Bum Lee, M. Aruni DeSilva, Mauricio Quiroz-Guzman, William F. Schneider and Joan F. Brennecke, "Competing Reactions of CO_2 with Cations and Anions in Azolide Ionic Liquids," ChemSusChem, 2014, 7(7), 1970-1975.
3. Samuel Seo, Mauricio Quiroz-Guzman, Aruni DeSilva, Tae Bum Lee, Yong Huang, Brett F. Goodrich, William F. Schneider, and Joan F. Brennecke, "Chemically Tunable Ionic Liquids with Aprotic Heterocyclic Anions (AHAs) for CO_2 Capture," J. Phys. Chem. B, 2014, 118, p. 5740-5751. DOI 10.1021/jp502279w.
4. Samuel Seo, M. Aruni DeSilva and Joan F. Brennecke, "Physical Properties and CO_2 Reaction Pathway of 1-Ethyl-3-Methylimidazolium Ionic Liquids with Aprotic Heterocyclic Anions," J. Phys. Chem. B., 2014, 118 (51), pp 14870-14879.
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7. Ramesh Singh, Eliseo Marin-Rimoldi and Edward J. Maginn, "A Monte Carlo Simulation Study To Predict the Solubility of Carbon Dioxide, Hydrogen, and Their Mixture in the Ionic Liquids 1‑Alkyl-3-methylimidazolium bis(trifluoromethanesulfonyl)amide ([Cnmim+][Tf2N−], n = 4, 6)", Industrial and Engineering Chemistry Research, 2015, 54, 4385-4395.
8. Samir Budhathoki, Jindal K. Shah and Edward J. Maginn, "Molecular Simulation Study of the Solubility, Diffusivity and Permselectivity of Pure and Binary Mixtures of CO_2 and CH_4 in the Ionic Liquid 1-*n*-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide", *Industrial and Engineering Chemistry Research*, **2015**, 54, 8821–8828
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10. T. B. Lee, S. Oh, T. R. Gohndrone, O. Morales-Collazo, S. Seo, J. F. Brennecke, and W. F. Schneider, "CO_2 Chemistry of Phenolate-Based Ionic Liquids," *J. Phys. Chem. B* **2016**, *120*, 1509–1517.
11. Bo Hong, Luke D. Simoni, Joshua E. Bennett, Joan F. Brennecke, and Mark A. Stadtherr. "Simultaneous Process and Material Design for Aprotic N-Heterocyclic Anion Ionic Liquids in Post-Combustion CO2 Capture, submitted for publication (2016).

Presentations

1. B. Hong, J. E. Bennett, J. F. Brennecke, and M. A. Stadtherr, "Chemically-Complexing Ionic Liquids for Pre-Combustion CO_2 Capture: Design of Chemical Properties," AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.

2. Joan F. Brennecke,"CO_2 Separations with Liquid Absorbents," Department of Chemical Engineering, University of California at Berkeley, Feb. 28, 2013.
3. Joan F. Brennecke, Thomas R. Gohndrone, Mauricio Quiroz-Guzman, and M. Aruni DeSilva, "Reaction Chemistry of Phosphonium and Ammonium Ionic Liquids with AHA Anions for CO_2 Capture," American Chemical Society, Indianapolis, IN, Sept. 10, 2013.
4. Joan F. Brennecke, plenary lecture, "Ionic Liquids for CO_2 Capture," 50 Years of Post Graduate Education in Chemical Engineering in Brazil, Federal University of Rio de Janeiro, October 24, 2013.
5. Joan F. Brennecke, "Reaction Chemistry of Ionic Liquids for CO_2 Capture," Colorado School of Mines, January 17, 2014.
6. Joan F. Brennecke, "Designing Ionic Liquids for CO_2 Capture," Texas Tech University, January 24, 2014.
7. Joan F. Brennecke, "Ionic Liquids in Industrial and Engineering Chemistry," E. V. Murphree Award address, 247th National Meeting of the American Chemical Society, Dallas, TX, March 19, 2014.
8. Joan F. Brennecke, Ashton Cary Lectures, "Using Ionic Liquids for Energy Applications" and "Effect of Cation, Water and Other Additives on AHA Ionic Liquids for CO_2 Capture," Georgia Institute of Technology, April 23 and 24, 2014.
9. Joan F. Brennecke, Katz Award Lecture and Levich Institute Lecture, "Designing Ionic Liquids for CO_2 Capture" and "Tuning the Properties of Ionic Liquids and Ionic Liquid Mixtures," City College of New York, April 28 and 29, 2014.
10. Joan F. Brennecke, "Thermodynamics of Mixtures of Ionic Liquids and Gases," US Poland Workshop on the Thermodynamics of Complex Fluids and Interfaces," Warsaw, Poland, June 13, 2014.
11. Samuel Seo and Joan F. Brennecke, Keynote Speaker, "The Effect of Additives and Cation-Anion Association on CO_2 Uptake by AHA Ionic Liquids," ILSEPT-2nd International Conference on Ionic Liquids in Separation and Purification Technology, Toronto, Canada, June 29-July 2, 2014.
12. Joan F. Brennecke, Global Climate and Energy Project (GCEP) Distinguished Lectures, "CO_2 Removal with Ionic Liquids," Bank of America August 1, 2014; Exxon-Mobil August 4, 2014; GE August 22, 2014; DuPont August 25, 2014.
13. Joan F. Brennecke, The Fred Kavli Innovations in Chemistry Lecture, "How Ionic Liquids Can Contribute to Global Stewardship," ACS National Meeting, San Francisco, CA, August 11, 2014.
14. Joan F. Brennecke, "Ionic Liquids for CO_2 Capture: Chemisty, Cosolvents and Ionicity," Gordon Research Conference," August 17-22, 2014.
15. Joan F. Brennecke, "Ionic Liquids for Post-Combustion CO_2 Capture," Andlinger Center for Energy and the Environment, Princeton University, January 16, 2015.
16. Joan F. Brennecke, Institute for Materials Research Distinguished Lecture Series, "Ionic Liquids for Post-Combustion CO2 Capture," Ohio State University, February 18, 2015.
17. Joan F. Brennecke, Symposium in Honor of Charlie Liotta, "Reaction Chemistry of Ionic Liquids with CO_2 for Post-Combustion Capture," Department of Chemisty, Georgia Institute of Technology, February 26, 2015.
18. Joan F. Brennecke, "Using Ionic Liquids for Post-Combustion Carbon Capture," Department of Chemical Engineering, University of Washington, April 27, 2015.
19. Joan F. Brennecke, Samuel Parr Lecture, Carbon Capture with Ionic Liquids, Department of Chemical Engineering, University of Illinois at Urbana-Champaign, May 7, 2015.
20. Thomas R. Gohndrone, Burcu E. Gurkan, Mauricio Quiroz-Guzman, M. Aruni DeSilva, Joan F. Brennecke, "Reaction Kinetics and Mechanism Study: Reaction of Phosphonium Based Amine-Functionalized Ionic Liquids with CO_2," 5th Congress on Ionic Liquids, Algarve, Portugal, April 21-25, 2013.
21. M. Aruni DeSilva, Samuel Seo, Chaojun Shi, Marjorie Massel and Joan F. Brennecke, "Investigation of Reactivity of Imidazolium Based Aprotic Heterocyclic Anion (AHA) Ionic Liquids Using," (poster and 'flash' presentation), 5th Congress on Ionic Liquids, Algarve, Portugal, April 21-25, 2013.
22. Mauricio Quiroz-Guzman, M. Aruni DeSilva and Joan F.Brennecke, "Ionic liquids with Aprotic Heterocyclic Anions and their reactivity with water and CO_2," (poster presentation), 5th Congress on Ionic Liquids, Algarve, Portugal, April 21-25, 2013.
23. Joshua Bennett, Aruni DeSilva and Joan F. Brennecke, "Molar Volume Dependence of N_2 Solubility in Ionic Liquids," AIChE Meeting, San Francisco, CA, Nov. 3-8, 2013.

24. Thomas Gohndrone and Joan F. Brennecke, "Temperature and Pressure Effect on the Capture of CO2 with Phosphonium Based Ionic Liquids," poster presentation, ILSEPT-2nd International Conference on Ionic Liquids in Separation and Purification Technology, Toronto, Canada, June 29-July 2, 2014.
25. Edward J. Maginn, "Developing New Materials for Energy and Environmental Applications via Molecular Simulation", Department of Chemical and Biological Engineering, Colorado School of Mines, Oct. 4, 2013.
26. Edward J. Maginn, "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.
27. Edward J. Maginn, "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.
28. Edward J. Maginn, "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.
29. 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.
30. Brandon L. Ashfeld. "From Carbon to Cancer: The Impact of Reaction Development on Natural Products and Designed Materials Synthesis." Department of Chemistry and Biochemistry, Hope College, Holland, MI. November 6, 2015.
31. Brandon L. Ashfeld. "From Carbon to Cancer: The Impact of Reaction Development on Natural Products and Designed Materials Synthesis." Department of Chemistry and Biochemistry, Calvin College, Grand Rapids, MI. November 5, 2015.
32. Brandon L. Ashfeld. "Nitrene and Carbene Surrogates: New Methods in C–N and C–C Bond Formation for Heterocycle Construction." 249th American Chemical Society National Meeting and Symposium, Denver, CO. March 25, 2015.
33. Brandon L. Ashfeld. "Nitrene and Carbene Surrogates: New Methods in C–N and C–C Bond Formation for Heterocycle Construction." 248th American Chemical Society National Meeting and Symposium, San Francisco, CA. August 16, 2014.
34. Brandon L. Ashfeld. "Nitrene and Carbene Surrogates: New Methods in C–N and C–C Bond Formation for Heterocycle Construction." 51st Gordon Research Conference on Heterocyclic Compounds, Salve Regina University, Newport, RI. June 17, 2014.
35. Brandon L. Ashfeld. "Chemoselective Nucleophilic Substitution Strategies Toward Natural Products and Designed Materials." University of Notre Dame, Notre Dame, IN. October 23, 2013.
36. Brandon L. Ashfeld. "Novel Diarylheptanoids for the Treatment of Glioblastoma Multiforme." Concepts to Clinic Meeting, Riley Hospital Children's Clinical Research Center, Indianapolis, IN. September 20, 2013.
37. Brandon L. Ashfeld. "Harnessing Masked Electrophilicity and Nucleophilicity: Alternative Strategies for Selective C–C and C–N Bond Formations." Young Academic Investigators Award Symposium, 246th American Chemical Society National Meeting and Exposition, Indianapolis, IN. September 9, 2013.
38. Brandon L. Ashfeld. "Maximizing Chemoselectivity and Convergency in the Strategic Assembly of Biologically Active Natural Products." University of Illinois at Chicago, Chicago, IL. May 31, 2013.
39. Brandon L. Ashfeld. "Chemoselective Nucleophilic Substitution Strategies Toward Natural Products and Designed Materials." Northwestern University, Evanston, IL. May 30, 2013.
40. Brandon L. Ashfeld. "Exploiting Unconventional Carbonyl Reactivity for Natural Products and Designed Materials Synthesis." Columbia University, New York, NY. April 24, 2013.
41. Brandon L. Ashfeld. "New Strategies in Chemoselective Carbonyl Functionalization." New York University, New York, NY. April 23, 2013.
42. Brandon L. Ashfeld. "Maximizing Chemoselectivity and Convergency in the Strategic Assembly of Biologically Active Natural Products." Massachusetts Institute of Technology, Cambridge, MA. April 11, 2013.
43. Brandon L. Ashfeld. "How New Synthetic Methods Enable the Design of Brain and Nervous System

Cancer Chemotherapies." Interdisciplinary Science Seminar, SCPP 23100. University of Notre Dame, Notre Dame, IN. April 2, 2013.

44. Brandon L. Ashfeld. "Maximizing Chemoselectivity and Convergency in the Strategic Assembly of Biologically Active Natural Products." University of Texas at Austin, Austin, TX. March 29, 2013.
45. Brandon L. Ashfeld. "Exploiting Unconventional Carbonyl Reactivity for Natural Products and Designed Materials Synthesis." Texas A&M University, College Station, TX. March 28, 2013.
46. Brandon L. Ashfeld. "New Strategies in Chemoselective Carbonyl Functionalization." University of Texas Southwest Medical Center, Dallas, TX. March 26, 2013.
47. Brandon L. Ashfeld. "Maximizing Chemoselectivity and Convergency in the Strategic Assembly of Biologically Active Natural Products." Rutgers University, Piscataway, NJ. March 12, 2013.
48. Brandon L. Ashfeld. "New Strategies in Chemoselective Carbonyl Functionalization." Princeton University, Princeton, NJ. March 11, 2013.
49. Brandon L. Ashfeld. "Exploiting Unconventional Carbonyl Reactivity for Natural Products and Designed Materials Synthesis." Stanford University, Palo Alto, CA. February 20, 2013.
50. Brandon L. Ashfeld. "Harnessing Masked Electrophilicity and Nucleophilicity: Alternative Strategies for Selective C–C and C–N Bond Formations." Genentech, South San Francisco, CA. February 19, 2013.
51. Brandon L. Ashfeld. "Exploiting Unconventional Carbonyl Reactivity for Natural Products and Designed Materials Synthesis." University of Michigan, Ann Arbor, MI. January 17, 2013.
52. Brandon L. Ashfeld. "Harnessing Masked Electrophilicity: Alternative Strategies for Selective Carbonyl Functionalization." Wayne State University, Detroit, MI. January 16, 2013.
53. "Redox Phosphorus(V/III)-Mediated C–N and C–C Bond Formations." Justin D. Vail, Kevin X. Rodriguez, Erin E. Wilson, Jennifer L. Meloche, Antonio J. Lepore, Kaitlyn Eckert and Brandon L. Ashfeld. 62nd Organic Reactions and Process Gordon Research Conference, Bates College, Lewiston, ME. July 19-24, 2015 (poster presentation).
54. "New Methods in Heterocycle Construction: Natural Product and Designed Material Syntheses." Catherine A. Campos, Joseph B. Gianino, Lauren M. Fleury, Antonio J. Lepore, and Brandon L. Ashfeld. 49th Gordon Research Conference on Heterocyclic Compounds, Salve Regina University, Newport, RI. June 16-21, 2013 (poster presentation).
55. Monika Vogt, and Brandon L. Ashfeld "Carbon Dioxide Separation Using *N*-Heterocyclic Ionic Liquids and Carbenes." 5th Annual Chicago Organic Symposium. University of Notre Dame, Notre Dame, IN (Poster Presentation). July 12, 2013.
56. Monika Vogt, and Brandon L. Ashfeld "Carbon Dioxide Separation Using *N*-Heterocyclic Ionic Liquids and Carbenes." Graduate Student Union Symposium, University of Notre Dame, Notre Dame, IN (Poster Presentation). February 27, 2013.
57. T. B. Lee, T. R. Gohndrone, S. Seo, S. M. Oh, J. F. Brennecke, W. F. Schneider, "CO_2 capture chemistry of task-specific ionic liquids: Interplay between CO_2, cation, and anion" 6th International Congress of Ionic Liquids, June 16-20, 2015, Jeju, Korea
58. W. F. Schneider, "Design Principles for Reversible CO2 Chemistries," Rice University, Department of Chemical and Biomolecular Engineering, Houston, Texas, April 23, 2015.
59. W. F. Schneider, "Design Principles for Reversible CO2 Chemistries," American Chemical Society National Meeting, Denver, Colorado, March 25, 2015.
60. T. B. Lee, S. Seo, Q. Sheridan, T. R. Gohndrone, G. A. Bonilla, E. Maginn, J. F. Brennecke, W. F. Schneider, "CO_2 Capture Chemistry of Azolide-based Ionic Liquids: Interplay between CO_2, Ions, and Water" 250th ACS National Meeting and Exposition, August 16-20, 2015, Boston, MA

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