

## Krista S. Walton

Professor and Robert "Bud" Moeller Faculty Fellow  
School of Chemical & Biomolecular Engineering  
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### I. EARNED DEGREES

Ph.D. 2005 Chemical Engineering Vanderbilt University  
B.S.E. 2000 Chemical Engineering University of Alabama–Huntsville, *Magna Cum Laude*

### II. APPOINTMENTS

2018 – present Academic Program Director, Professional Master's in Manufacturing Leadership, College of Engineering, Georgia Institute of Technology  
2016 – present Professor and Robert "Bud" Moeller Faculty Fellow, Chemical & Biomolecular Engineering, Georgia Tech  
2014 – present Associate Editor, *Industrial & Engineering Chemistry Research*  
2012 – 2016 Associate Professor and McClatchey Faculty Fellow, Chemical & Biomolecular Engineering, Georgia Tech  
2009 – 2012 Assistant Professor, Chemical & Biomolecular Engineering, Georgia Tech  
2006 – 2009 Tim and Sharon Taylor Assistant Professor, Chemical Engineering, Kansas State University  
2005 – 2006 Postdoctoral Research Associate and ACS PRF Fellow, Northwestern University

### III. HONORS AND AWARDS

#### A. INTERNATIONAL OR NATIONAL AWARDS

2019 Selected to 2020-2022 cohort of the Defense Science Study Group (DSSG)  
2016 AIChE FRI/John G. Kunesh Award for Excellence in Separations Research  
2015 University of Alabama-Huntsville Alumni of Achievement Award  
2015 ACS Women Chemists Committee Rising Star Award  
2015 UAH College of Engineering Distinguished Speaker  
2013 International Adsorption Society Award for Excellence in Publications by a Young Member of the Society (*Inaugural Award*)  
2012 Kavli Fellow, National Academy of Sciences (NAS) German-American Frontiers of Science Symposium (GAFOS), Meeting Chair (U.S. side)  
2011 Young Scientist Delegation, IAP/World Economic Forum's "Summer Davos" in Dalian, People's Republic of China, Invitee (1 of 2 US Young Scientists chosen after nomination by the US National Academies)  
2011 Kavli Fellow and Organizer, National Academy of Sciences (NAS) German-American Frontiers of Science Symposium (GAFOS)  
2009 CAREER Award, National Science Foundation  
2008 Presidential Early Career Award for Scientists and Engineers (PECASE)  
2007 Army Research Office Young Investigator Program (YIP) Award  
2005 American Chemical Society Petroleum Research Fund Alternative Energy Postdoctoral Fellowship  
2005 AIChE Separations Division Graduate Research Award, Adsorption and Ion Exchange  
2000 IBM Graduate Fellowship

**B. INSTITUTE OR SCHOOL AWARDS**

- 2015 Georgia Power Professor of Excellence, College of Engineering
- 2013 Georgia Tech CETL Class of 1940 Course Survey Teaching Effectiveness Award
- 2009 Sigma Xi Outstanding Junior Scientist Award, KSU
- 1999 Society of Women Engineers Student Engineer of the Year, Alabama
- 1999 Alabama Association of Colleges & Employers Cooperative Education Student of the Year
- 1999 UAH Cooperative Education Student of the Year

**IV. RESEARCH, SCHOLARSHIP, AND CREATIVE ACTIVITIES****A. PUBLISHED BOOKS, BOOK CHAPTERS, AND EDITED VOLUMES****A1. Books**

Beaudet, R. A., Bandosz, T. J., Berkowitz, J. B., Clack, H. L., Gekler, W. C., Koller, L. D., LeVan, M. D., Pendergrass, J. A., Walton, K. S., Weber, W. J., Jr., and Yang, Y.-C., National Research Council. *The Disposal of Activated Carbon from Chemical Agent Disposal Facilities, Board on Army Science and Technology*. Washington, D. C., National Academies Press, 2009.

**A2. Book Chapters**

1. Dubbeldam, D. and Walton, K. S., "On the Application of Classical Molecular Simulations of Adsorption in Metal-Organic Frameworks" Book chapter in *Metal-Organic Frameworks: Materials Modeling towards Engineering Applications* edited by Jiang Jianwen (Pan Stanford Publishing Pte Ltd, 2013).
2. LeVan, M. D., Carta, G., Ritter, J. A., Walton, K. S., "Adsorption and Ion Exchange", Chapter 16 in *Perry's Chemical Engineers' Handbook*, 9<sup>th</sup> edition, (McGraw-Hill, 2019).
3. Walton, K. S., "Water Stability of Metal-Organic Frameworks," Chapter 8 in *Gas Adsorption in Metal-Organic Frameworks: Fundamentals and Applications*, edited by T. Grant Glover and Bin Mu (CRC Press Taylor & Francis Group, 2019)

**B. REFEREED PUBLICATIONS AND SUBMITTED ARTICLES (h-index = 43)****B1. Published and Accepted Journal Articles (Advisees in bold)****Ph.D. Research:**

1. Walton, K. S., and M. D. LeVan. Consistency of Energy and Material Balances for Bidisperse Particles in Fixed-Bed Adsorption and Related Applications. *Industrial & Engineering Chemistry Research*, 2003, 42, 6938–6948.
2. Walton, K. S., G. Pigorini, and M. D. LeVan. Simple Group Contribution Theory for Adsorption of Alkanes in Nanoporous Carbons. *Chemical Engineering Science*, 2004, 59, 4425–4432.
3. Walton, K. S., and M. D. LeVan. Adsorbed-Phase Heat Capacities: Thermodynamically Consistent Values Determined from Temperature-Dependent Equilibrium Models. *Industrial & Engineering Chemistry Research*, 2005, 44, 178-182.
4. Walton, K. S., and M. D. LeVan. Development of Energy Balances for Fixed-Bed Adsorption Processes: Thermodynamic Paths, Heat Capacities, and Isosteric Heats. *Adsorption*, 2005, 11, 555-559.

5. Walton, K. S., and M. D. LeVan. Effect of Energy Balance Approximations on Simulation of Fixed-Bed Adsorption. *Industrial & Engineering Chemistry Research*, 2005, 44, 7474–7480.
6. Walton, K. S., C. L. Cavalcante Jr., and M. D. LeVan. Adsorption Equilibrium of Alkanes on a High Surface Area Activated Carbon Prepared from Brazilian Coconut Shells. *Adsorption*, 2005, 11, 107–111.
7. Walton, K. S., C. L. Cavalcante Jr., and M. D. LeVan. Adsorption of Light Alkanes on Coconut Nanoporous Activated Carbon. *Brazilian Journal of Chemical Engineering*, 2006, 23, 551–561.
8. Walton, K. S., and M. D. LeVan. A Novel Adsorption Cycle for CO<sub>2</sub> Recovery: Experimental and Theoretical Investigations of a Temperature Swing Compression Process. *Separation Science and Technology*, 2006, 41, 485–500.
9. Walton, K. S., and M. D. LeVan. Natural Gas Storage Cycles: Influence of Nonisothermal Effects and Heavy Alkanes. *Adsorption*, 2006, 12, 227–235.
10. Walton, K. S., M. B. Abney, and M. D. LeVan. Adsorption of CO<sub>2</sub> in Y and X Zeolites Modified by Alkali Metal Cation Exchange. *Microporous and Mesoporous Materials*, 2006, 91, 78–84.

#### Postdoctoral Research:

11. Düren, T., F. Millange, G. Férey, K. S. Walton, and R. Q. Snurr. Calculating Geometric Surface Areas as a Characterization Tool for Metal-Organic Frameworks. *Journal of Physical Chemistry C*, 2007, 111(42), 15350-15356.
12. Dubbeldam, D., H. Frost, K. S. Walton, D. E. Ellis, and R. Q. Snurr. Molecular Simulation of Adsorption Sites of Light Gases in the Metal-Organic Framework IRMOF-1. *Fluid Phase Equilibria*, 2007, 261, 152-161.
13. Walton, K. S. and R. Q. Snurr. Applicability of the BET Method for Determining Surface Areas of Metal-Organic Frameworks. *Journal of the American Chemical Society*, 2007, 129, 8552-8556.
14. Dubbeldam, D., K. S. Walton, D. E. Ellis, and R. Q. Snurr. Exceptional Negative Thermal Expansion in Metal-Organic Frameworks. *Angewandte Chemie*, 2007, 46, 4496-4499.
15. Walton, K. S., A. R. Millward, D. Dubbeldam, H. Frost, J. J. Low, O. M. Yaghi, and R. Q. Snurr. Understanding Inflections and Steps in Carbon Dioxide Adsorption Isotherms in Metal-Organic Frameworks. *Journal of the American Chemical Society*, 2008, 130, 406-407.
16. Akbar, S., M. Pukala, and K. S. Walton. Adsorption of Aqueous Solutions of Carboxylic Acids on Montmorillonite, Silicalite, H-ZSM-5 and their Na<sup>+</sup> and Li<sup>+</sup> Exchanged Forms, *Journal of the Chemical Society of Pakistan*, 2008, 30, 546-548.

#### Walton Research Group:

17. Dubbeldam, D., C. J. Galvin, K. S. Walton, D. E. Ellis, and R. Q. Snurr. Separation and Molecular-level Segregation of Complex Alkane Mixtures using Metal-Organic Frameworks, *Journal of the American Chemical Society*, 2008, 130, 10884-10885.
18. Karra, J. R. and K. S. Walton. Effect of Open Metal Sites on Adsorption of Polar and Nonpolar Molecules in Metal-Organic Framework Cu-BTC, *Langmuir*, 2008, 24, 8620-8626.
19. Mu, B., F. Li, K. S. Walton. A Novel Metal-Organic Coordination Polymer for Selective Adsorption of CO<sub>2</sub> over CH<sub>4</sub>, *Chemical Communications*, 2009, 2493-2495.

20. Bae, Y.-S., D. Dubbledam, A. Nelson, K. S. Walton, J. T. Hupp, R. Q. Snurr. Strategies for Characterization of Large-pore Metal-Organic Frameworks by Combined Experimental and Computational Methods, *Chemistry of Materials*, 2009, 21, 4768-4777.
21. **Mu**, B., P. M. **Schoenecker**, K. S. Walton. Gas Adsorption Study on Mesoporous Metal-Organic Framework UMCM-1, *Journal of Physical Chemistry C*, 2010, 114, 6464-6471.
22. **Mu**, B., Y. **Huang**, K. S. Walton. A Metal-Organic Framework with Coordinatively Unsaturated Centers and Nanoporous Structure, *CrystEngComm*, 2010, 12, 2347-2349. (*New Talent themed issue*).
23. **Karra**, J. R. and K. S. Walton. Molecular Simulations and Experimental Studies of CO<sub>2</sub>, CO, and N<sub>2</sub> Adsorption in Metal-Organic Frameworks, *Journal of Physical Chemistry C*, 2010, 114, 15735-15740.
24. **Huang**, Y., B. **Mu**, P. M. **Schoenecker**, C. G. **Carson**, J. R. **Karra**, Y. **Cai**, and K. S. Walton. A Porous Flexible Homochiral Array of Single-Stranded Helical Nanotubes Exhibiting Single-Crystal-to-Single-Crystal Oxidation Transformation, *Angewandte Chemie*, 2011, 50, 436-440.
25. **Mu**, B. and K. S. Walton. High Pressure Adsorption Equilibrium of CO<sub>2</sub>, CH<sub>4</sub>, and CO in an Impregnated Carbon, *Journal of Chemical & Engineering Data*, 2011, 56, 390-397.
26. **Mu**, B. and K. S. Walton. Adsorption Equilibrium of Methane and Carbon Dioxide on Porous Metal-Organic Framework Zn-BTB, *Adsorption*, 2011, 17, 777-782.
27. Lu, G., O. K. Farha, L. E. Kreno, P. M. **Schoenecker**, K. S. Walton, R. P. Van Duyne, and J. T. Hupp. Fabrication of Metal-Organic-Framework-containing Silica-Colloidal Crystals for Vapor Sensing, *Advanced Materials*, 2011, 38, 4449-4452.
28. **Mu**, B. and K. S. Walton. Thermal Analysis and Heat Capacity Study of Metal-Organic Frameworks, *Journal of Physical Chemistry C*, 2011, 115, 22748-22754.
29. **Schoenecker**, P. M., C. G. **Carson**, H. **Jasuja**, C. J. J. **Flemming**, and K. S. Walton. Effect of Water Adsorption on Retention of Structure and Surface Area of Metal-Organic Frameworks, *Industrial & Engineering Chemistry Research*, 2012, 51 (18), 6513-6519.
30. **Mu**, B. and K. S. Walton. Breathing Effects of CO<sub>2</sub> Adsorption on a Flexible 3D Lanthanide Metal-Organic Framework, *Journal of Materials Chemistry*, 2012, 22(20), 10172-10178. (Invited, special issue "Integrating Functionality into Metal-Organic Frameworks").
31. **Han**, S., Y.-G. **Huang**, T. Watanabe, K. S. Walton, S. Nair, D. S. Sholl, and C. Meredith. High-Throughput Screening of Metal Organic Frameworks (MOFs) for CO<sub>2</sub> Separation, *ACS Combinatorial Science*, 2012, 14, 263-267.
32. **Cai**, Y., Y. Zhang, Y.-G. **Huang**, S. Marder, and K. S. Walton. Impact of Alkyl-Functionalized BTC on Properties of Copper-Based Metal-Organic Frameworks, *Crystal Growth & Design*, 2012, 12 (7), 3709-3713.
33. **Vilhelmsen**, L., K. S. Walton, and D. S. Sholl. Structure and Mobility of Metal Clusters in MOFs: Au, Pd, and AuPd clusters in MOF-74, *Journal of the American Chemical Society*, 2012, 134(30), 12807-12816.
34. **Jasuja**, H., Y.-G. **Huang**, and K. S. Walton, Adjusting the Stability of Metal-Organic Frameworks under Humid Conditions by Ligand Functionalization, *Langmuir*, 2012, 28(49), 16874-16880.
35. **Jasuja**, H., J. Zang, D. S. Sholl, and K. S. Walton. Rational Tuning of Water Vapor and CO<sub>2</sub> Adsorption in Highly Stable Zr-Based MOFs, *Journal of Physical Chemistry C*, 2012, 116(44), 23526-23532.

36. **Cmarik**, G. E., M. Kim, S. M. Cohen, and K. S. Walton. Turning the Adsorption Properties of UiO-66 via Ligand Functionalization, *Langmuir*, 2012, 28(44), 15606-15613.
37. **Karra**, J. R., B. E. **Grabicka**, Y.-G. **Huang**, and K. S. Walton. Adsorption Study of CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>, and H<sub>2</sub>O on an Interwoven Copper Carboxylate Metal-Organic Framework (MOF-14), *Journal of Colloid and Interface Science*, 2013, 392, 331-336.
38. **Jasuja**, H., N. C. **Burtch**, Y.-G. **Huang**, Y. **Cai**, K. S. Walton. Kinetic Water Stability of an Isostructural Family of Zinc-Based Pillared Metal-Organic Frameworks, *Langmuir*, 2013, 29(2), 633-642.
39. **Karra**, J. R., Y.-G. **Huang**, K. S. Walton. Synthesis, Characterization, and Adsorption Studies of Nickel (II), Zinc (II), and Magnesium (II) Coordination Frameworks of BTTB, *Crystal Growth & Design*, 2013, 13(3), 1075-1081.
40. DeCoste, J. B., G. W. Peterson, H. **Jasuja**, T. G. Glover, Y. -G. **Huang**, and K. S. Walton. Stability and Degradation Mechanisms of Metal-Organic Frameworks Containing Zr<sub>6</sub>O<sub>4</sub>(OH)(4) Secondary Building Unit, *Journal of Materials Chemistry A*, 2013, 1(18), 5642-5650.
41. **Jasuja**, H. and K. S. Walton, Effect of Catenation and Basicity of Pillared Ligands on the Water Stability of MOFs, *Dalton Transactions*, 2013, 42(43), 15421-15426.
42. **Jasuja**, H. and K. S. Walton. Experimental Study of CO<sub>2</sub>, CH<sub>4</sub>, and Water Vapor Adsorption on a Dimethyl-Functionalized UiO-66 Framework, *Journal of Physical Chemistry C*, 2013, 117(14), 7062-7068.
43. **Burtch**, N. C., H. **Jasuja**, D. Dubbeldam, and K. S. Walton, Molecular-Level Insight into Unusual Low Pressure CO<sub>2</sub> Affinity in Pillared Metal-Organic Frameworks, *Journal of the American Chemical Society*, 2013, 135(19), 7172-7180.
44. **Han**, S., Y. -G. **Huang**, T. **Watanabe**, S. Nair, K. S. Walton, D. S. Sholl, and J. C. Meredith. MOF Stability and Gas Adsorption as a Function of Exposure to Water, Humid Air, SO<sub>2</sub>, and NO<sub>2</sub>, *Microporous and Mesoporous Materials*, **2013**, 173, 86-91.
45. **Schoenecker**, P. M., G. A. **Belancik**, B. E. **Grabicka**, and K. S. Walton, Kinetic Study and Crystallization Process Design for Scale-Up of UiO-66-NH<sub>2</sub> Synthesis, *AIChE Journal*, 2013, 59(4), 1255-1262.
46. Peterson, G. W., J. B. DeCoste, T. G. Glover, Y.-G. **Huang**, H. **Jasuja**, and K. S. Walton. Effects of Pelletization Pressure on the Physical and Chemical Properties of the Metal-Organic Frameworks Cu<sub>3</sub>(BTC)<sub>2</sub> and UiO-66. *Microporous and Mesoporous Materials*, 2013, 179, 48-53.
47. Dubbeldam, D., A. Torres-Knoop, K. S. Walton, On the Inner Workings of Monte Carlo Codes, *Molecular Simulation*, 2013, 39(14-15), 1253-1292.
48. Walton, K. S. Recognizing the Unrecognizable, *Nature Chemistry*, 2014, 6, 277-278.
49. **Mangarella**, M. C., J. L. Ewbank, M. R. **Dutzer**, F. M. Alamgir, and K. S. Walton. Synthesis of Embedded Iron Nanoparticles in Fe<sub>3</sub>C-Derived Carbons, *Carbon*, 2014, 79, 74-84.
50. **Burtch**, N. C., H. **Jasuja**, K. S. Walton, Water Stability and Adsorption in Metal-Organic Frameworks, *Chemical Reviews*, 2014, 114, 10575-10612.

51. **Cai, Y.**, A. R. Kulkarni, Y.-G. **Huang**, D. S. Sholl, K. S. Walton, Control of Metal-Organic Framework Crystal Topology by Functionalization: Functionalized HKUST-1 Derivatives, *Crystal Growth & Design*, 2014, 14, 6122-6128.
52. **Tulig, K.** and K. S. Walton, An Alternative UiO-66 Synthesis for HCl-Sensitive Nanoparticle Encapsulation, *RSC Advances*, 2014, 4, 51080-51083.
53. **Jasuja, H.**, Y. **Jiao**, N. C. **Burtch**, Y.-G. **Huang**, and K. S. Walton, Synthesis of Cobalt, Nickel, Copper, and Zinc-based Water Stable Pillared Metal-Organic Frameworks, *Langmuir*, 2014, 30, 14300-14307.
54. **Jasuja, H.**, G. W. Peterson, J. B. Decoste, M. A. Brow, and K. S. Walton, Evaluation of MOFs for Air Purification and Air Quality Control Applications: Ammonia Removal from Air, *Chemical Engineering Science*, 2015, 124, 118-124.
55. **Mounfield, W.**, K. S. Walton, Effect of Synthesis Solvent on the Breathing Behavior of MIL-53(Al), *Journal of Colloid and Interface Science*, 2015, 447, 33-39.
56. **Karra, J.R.**, H. **Jasuja**, Y.-G. **Huang**, K. S. Walton, Structural Stability of BTTB-based Metal-Organic Frameworks under Humid Conditions, *Journal of Materials Chemistry A*, 2015, 3, 1624-1631.
57. **Burtch, N. C.**, A. Torres-Knoop, G. S. Foo, J. Leisen, C. Sievers, B. Ensing, D. Dubbeldam, K. S. Walton, Understanding DABCO Nanorotor Dynamics in Isostructural Metal-Organic Frameworks, *Journal of Physical Chemistry Letters*, 2015, 6, 812-816.
58. **Burtch, N. C.**, D. Dubbeldam, K. S. Walton, Investigating Water and Framework Dynamics in Pillared MOFs, *Molecular Simulation*, 2015, 41, 1379-1387.
59. Walton, K. S., Movies of a Growth Mechanism, *Nature*, 2015, 523, 535-536.
60. Walton, K. S., D. S. Sholl, Predicting Multi-Component Adsorption: 50 Years of the Ideal Adsorbed Solution Theory, *AIChE Journal*, 2015, 61, 2757-2762.
61. **Burtch, N. C.**, K. S. Walton, Modulating Adsorption and Stability Properties in Pillared Metal-Organic Frameworks: A Model System for Understanding Ligand Effects, *Account of Chemical Research*, 2015, 48, 2850-2857.
62. **Mangarella, M. C.**, K. S. Walton, Tailored Fe<sub>3</sub>C-Derived Carbons with Embedded Fe Nanoparticles for Ammonia Adsorption, *Carbon*, 2015, 95, 208-219.
63. **Jiao, Y.**, C. R. **Morelock**, N. C. **Burtch**, W. P. **Mounfield**, J. T. **Hungerford**, K. S. Walton, Tuning the Kinetic Water Stability and Adsorption Interactions of Mg-MOF-74 by Partial Substitution with Co or Ni, *Industrial & Engineering Chemistry Research*, 2015, 54, 12408-12414.
64. **Mounfield, W. P.**, U. Tumuluri, Y. **Jiao**, M. Li, S. Dai, Z. Wu, K. S. Walton, Role of Defects and Metal Coordination on Adsorption of Acid Gases in MOFs and Metal Oxides: An In Situ IR Spectroscopic Study, *Microporous and Mesoporous Materials*, 2016, 227, 65-75.
65. **Durante, L.**, K. S. Walton, D. S. Sholl, C. W. Jones, CO<sub>2</sub> Capture via Adsorption in Amine-Functionalized Sorbents, *Current Opinion in Chemical Engineering*, 2016, 12, 82-90.
66. Torres-Knoop, A., N. C. **Burtch**, A. Poursaeidesfahani, S. P. Balaji, R. Kools, F. Smit, K. S. Walton, T. Vlugt, D. Dubbeldam, Optimization of Particle Transfers in the Gibbs Ensemble for Systems with Strong and Directional Interactions Using CBMC, CFCMC, and CB/CFCMC, *Journal of Physical Chemistry C*, 2016, 120, 9148-9159.

67. **Mounfield, W. P., M. Taboraga Claire, P. K. Agrawal, C. W. Jones, K. S. Walton**, Synergistic Effect of Mixed Oxide on the Adsorption of Ammonia with Metal-Organic Frameworks, *Industrial & Engineering Chemistry Research*, 2016, 55, 6492-6500.
68. Qu, C., Y. **Jiao**, B. Zhao, D. Chen, R. Zou, K. S. Walton, M. Liu, Design and Synthesis of Kinetically Stable, Pillared MOFs for High-performance Supercapacitors, *Nano Energy*, 2016, 26, 66-73.
69. **Darunte, L. A., A. D. Oetomo**, K. S. Walton, D. S. Sholl, C. W. Jones, Direct Air Capture of CO<sub>2</sub> Using Amine Functionalized MIL-101(Cr), *ACS Sustainable Chemistry Engineering*, 2016, 4, 5761-5768.
70. Heinen, J., **N. C. Burtch**, K. S. Walton, C. F. Guerra, D. Dubbeldam, Predicting Multicomponent Adsorption Isotherms in Open-Metal Site Materials Using Force Field Calculations Based on Energy Decomposed Density Functional Theory, *Chemistry European Journal*, 2016, 22, 18045-18050.
71. **Mounfield, W. P.**, C. Han, S. H. Pang, U. Tumuluri, **Y. Jiao**, S. Bhattacharyya, **M. R. Dutzer**, S. Nair, Z. Wu, R. P. Lively, D. S. Sholl, K. S. Walton, Synergistic Effects of Water and SO<sub>2</sub> on Degradation of MIL-125 in the Presence of Acid Gases, *Journal of Physical Chemistry C*, 2016, 120, 27230-27240.
72. Bhattacharyya, S., S. Pang, **M. R. Dutzer**, R. P. Lively, K. S. Walton, D. S. Sholl, S. Nair, Interactions of SO<sub>2</sub>-Containing Acid Gases with ZIF-8: Structural Changes and Mechanistic Investigations, *Journal of Physical Chemistry C*, 2016, 120, 27222-27229.
73. **Joshi, J. N., E. Y. Garcia-Gutierrez, C. M. Moran, J. I. Deneff**, K. S. Walton, Engineering Copper Carboxylate Functionalities on Water Stable Metal-Organic Frameworks for Enhancement of Ammonia Removal Capacities, *Journal of Physical Chemistry C*, 2017, 121, 3310-3319.
74. **Moran, C. M.**, R. M. Marti, S. E. Hayes, K. S. Walton, Synthesis and Characterization of Aluminum Carbide-Derived Carbon with Residual Aluminum-Based Nanoparticles, *Carbon*, 2017, 114, 482-495.
75. Howe, J., **C. R. Morelock, Y. Jiao**, K. Chapman, K. S. Walton, D. S. Sholl, Understanding Structure, Metal Distribution, and Water Adsorption in Mixed-Metal MOF-74, *Journal of Physical Chemistry C*, 2017, 121, 627-635.
76. Zhang, D., **M. R. Dutzer**, T. Liang, A. F. Fonseca, Y. Wu, K. S. Walton, D. S. Sholl, A. H. Farmahini, S. K. Bhatia, S. B. Sinnott, Computational Investigation on CO<sub>2</sub> Adsorption in Titanium Carbide-Derived Carbons with Residual Titanium, *Carbon*, 2017, 111, 741-751.
77. **Dutzer, M. R., M. C. Mangarella**, J. A. Schott, S. Dai, K. S. Walton, The Effects of Reactor Design on the Synthesis of Titanium Carbide-Derived Carbon, *Chemical Engineering Science*, 2017, 160, 191-199.
78. **Darunte, L. A.**, Y. Terada, **C. R. Murdock**, K. S. Walton, D. S. Sholl, C. W. Jones, Monolith Supported Amine Functionalized Mg<sub>2</sub>(dobpdc) Adsorbents for CO<sub>2</sub> Capture, *ACS Applied Materials & Interfaces*, 2017, 9, 17043-17051.
79. Heinen, J., **N. C. Burtch**, K. S. Walton, D. Dubbeldam, Flexible Force Field Parameterization through Fitting on the Ab Initio-Derived Elastic Tensor, *Journal of Chemical Theory and Computation*, 2017, 13, 3722-3730.

80. Tumuluri, U., J. D. Howe, **W. P. Mounfield III**, M. Li, M. Chi, Z. D. Hood, K. S. Walton, D. S. Sholl, S. Dai, Z. Wu, Effect of Surface Structure of TiO<sub>2</sub> Nanoparticles on CO<sub>2</sub> Adsorption and SO<sub>2</sub> Resistance, *ACS Sustainable Chemistry & Engineering*, 2017, 5, 9295-9306.
81. Demir, H., K. S. Walton, D. S. Sholl, Computational Screening of Functionalized UiO-66 Materials for Selective Contaminant Removal from Air, *Journal of Physical Chemistry C*, 2017, 121, 20396-20406.
82. Qu, Chong, B. T. Zhao, **Y. Jiao**, D. C. Chen, S. G. Dai, B. M. Deglee, Y. Chen, K. S. Walton, R. Q. Zou, M. L. Liu. Functionalized Bimetallic Hydroxides Derived from Metal-Organic Frameworks for High-Performance Hybrid Supercapacitor with Exceptional Cycling Stability, *ACS Energy Letters*, 2017, 2, 1263-1269.
83. **Jiao, Y.**, Y. Liu, G. Zhu, **J. T. Hungerford**, S. Bhattacharyya, R. P. Lively, D. S. Sholl, K. S. Walton, Heat-Treatment of Defective UiO-66 from Modulated Synthesis: Adsorption and Stability Studies, *Journal of Physical Chemistry C*, **\*ACS Editors' Choice**, 2017, 121, 23471-23479.
84. Walton, K. S. and D. S. Sholl, Research Challenges in Developing Materials for Large-Scale Energy Applications, *Joule*, 2017, 1, 201-211.
85. Marti, R. M., J. D. Howe, **C. R. Morelock**, M. S. Conradi, K. S. Walton, D. S. Sholl, S. E. Hayes, CO<sub>2</sub> Dynamics in Pure and Mixed-Metal MOFs with Open Metal Sites, *Journal of Physical Chemistry C*, 2017, 121, 25778-25787.
86. Agrawal, M., S. Bhattacharyya, **Y. Huang**, K. C. Jayachandrababu, **C. R. Murdock**, J. A. Bentley, A. Rivas-Cardona, M. M. Mertens, K. S. Walton, D.S. Sholl, S. Nair, Liquid-Phase Multicomponent Adsorption and Separation of Xylene Mixtures by Flexible MIL-53 Adsorbents, *Journal of Physical Chemistry C*, 2018, 122, 386-397.
87. Bhattacharyya, S., R. Han, W. G. Kim, Y. D. Chiang, K. C. Jayachandrababu, **J. T. Hungerford**, **M. R. Dutzer**, C. Mas, K. S. Walton, D. S. Sholl, S. Nair, Acid Gas Stability of Zeolitic Imidazolate Frameworks: Generalized Kinetic and Thermodynamic Characteristics, *Chemistry of Materials*, 2018, 30, 4089-4101.
88. **Joshi, J. N.**, G. Zhu, J. J. Lee, **E. A. Carter**, C. W. Jones, R. P. Lively, K. S. Walton, Probing Metal-Organic Framework Design for Adsorptive Natural Gas Purification, *Langmuir*, 2018, 34, 8443-8450.
89. **Moran, C. M.**, **J. N. Joshi**, R. M. Marti, S. E. Hayes, K. S. Walton, Structured Growth of Metal-Organic Framework MIL-53(Al) from Solid Aluminum Carbide Precursor, *Journal of the American Chemical Society*, 2018, 140, 9148-9153.
90. Nguyen, H. G. T. et al., A Reference High-Pressure CO<sub>2</sub> Adsorption Isotherm for Ammonium ZSM-5 Zeolite: Results of an Interlaboratory Study, *Adsorption-Journal of the International Adsorption Society*, 2018, 24, 531-539.
91. **Hungerford, J. T.**, S. Bhattacharyya, U. Tumuluri, S. Nair, Z. Wu, K. S. Walton, DMOF-1 as a Representative MOF for SO<sub>2</sub> Adsorption in Both Humid and Dry Conditions, *Journal of Physical Chemistry C*, 2018, 122, 23493-23500.
92. Bhattacharyya, S., R. Han, **J. N. Joshi**, G. Zhu, R. P. Lively, K. S. Walton, D. S. Sholl, and Sankar Nair, Stability of Zeolitic Imidazolate Frameworks in NO<sub>2</sub>, *Journal of Physical Chemistry C*, 2019, 123, 2336-2346.



93. **Darunte, L. A.**, T. Sen, C. Bhawanani, K. S. Walton, D. S. Sholl, M. J. Realff, C. W. Jones, Moving Beyond Adsorption Capacity in Design of Adsorbents for CO<sub>2</sub> Capture from Ultra-Dilute Feeds: Process Analysis of Adsorbents with Stepped Isotherms, *Industrial & Engineering Chemistry Research*, 2019, 58, 366-377.
94. Hossain, M. I., A. Udoh, **B. E. Grabicka**, K. S. Walton, S. M. C. Ritchie, T. G. Glover, Membrane Coated UiO-66 MOF Adsorbents, *Industrial & Engineering Chemistry Research*, 2019, 58, 1352-1362.
95. **Jiang, X., Y. Jiao, C. Moran**, X. W. Niew, **Y. T. Gong**, X. W. Guo, K. S. Walton, C. S. Song, CO<sub>2</sub> Hydrogenation to Methanol on Pd-Cu Bimetallic Catalysts with Lower Metal Loadings, *Catalysis Communications*, 2019, 118, 10-14.
96. **Hungerford, J. T.**, K. S. Walton, Room Temperature Synthesis of Metal-Organic Framework Isomers in the Tetragonal and Kagome Crystal Structure, *Inorganic Chemistry*, 2019, 58, 7690-7697.
97. **Deneff, J.I.**, K. S. Walton, Production of Metal-Organic Framework-Bearing Polystyrene Fibers by Solution Blow Spinning, *Chemical Engineering Science*, 2019, 203, 220-227.
98. **Hossain, M.**, J. D. Cunningham, T. M. Becker, B. E. Grabicka, K. S. Walton, B. D. Rabideau, T. G. Glover, Impact of MOF Defects on the Binary Adsorption of CO<sub>2</sub> and Water in UiO-66, *Chemical Engineering Science*, 2019, 203, 346-357.
99. **Joshi, J. N., C. M. Moran, H. P. Feininger, J. M. Dow**, K. S. Walton, Household Aluminum Products as Insoluble Precursors for Directed Growth of Metal-Organic Frameworks, *Crystal Growth & Design*, in press.

#### **B4. Submitted Journal Articles (Advisees in bold)**

100. **Burtch, N. C., I. Walton, C. R. Morelock, Y. Jiao**, J. Heinen, **J. T. Hungerford**, A. A. Yakovenko, W. Xu, D. Dubbeldam, K. S. Walton, In Situ Visualization of loading-dependent water effects in a stable metal-organic framework, *Nature Chemistry*, under review.
101. **Moran, C. M.**, R. M. Marti, **J. N. Joshi**, S. E. Hayes, K. S. Walton, Tuning Residual Metal in partially Etched Carbide-Derived Carbons for Enhanced Acid Gas Adsorption, *Carbon*, under review.

### **C. OTHER PUBLICATIONS AND CREATIVE PRODUCTS**

#### **C1. Patents**

Michael C. Mangarella and Krista S. Walton, Carbide-Derived Carbons having Incorporated Metal Chloride or Metallic Nanoparticles. US 9,833,765, United States Patent and Trademark Office, December 5, 2017.

**D. PRESENTATIONS****D1. Keynote Addresses and Plenary Lectures**

1. Keynote Speaker, International MOF Symposium, Dresden, Germany, September 16-17, 2013.
2. IAS Young Scientist Award Lecture, 11<sup>th</sup> Fundamentals of Adsorption Meeting, Baltimore, MD, May 19-24, 2013.
3. College of Engineering Distinguished Lecture, University of Alabama-Huntsville, "Engineering Next-Generation Materials for Environmental and Energy Applications," Huntsville, AL, January 30, 2015
4. Invited Award Lecture, Women Chemists Committee Rising Stars Awards Symposium, ACS Spring Meeting, Denver, CO, March 23, 2015.
5. Plenary Speaker, "Modulating Adsorption and Stability Properties in Pillared Metal-Organic Frameworks," 7<sup>th</sup> Pacific Basin Conference on Adsorption Science and Technology, Xiamen, China, September 24-27, 2015.
6. Keynote Speaker, "Metal-Organic Frameworks for Removal of Ammonia from Air," The 8<sup>th</sup> Sino-US Joint Conference of Chemical Engineering, Shanghai, China, October 12-16, 2015.
7. Keynote Speaker, "Impact of Metal Substitution on Stability and Adsorption Properties of MOF-74," ECI Separations Technology IX: Frontiers in Media, Techniques, and Technologies, Albufeira, Portugal, March 5-10, 2017.
8. Keynote Speaker, "Challenges in Developing Materials for Large-Scale Energy Applications," 1<sup>st</sup> Cutting Edge Symposium on the Current and Future Challenges of Energy Efficient Separation, Palm Cove, Australia, June 27-29, 2018.
9. Keynote Speaker, "Defect Engineering for Manipulating Porosity and Adsorption Behavior of Metal-Organic Frameworks," 8<sup>th</sup> Pacific Basin Conference on Adsorption Science and Technology, Sapporo, Japan, September 3-6, 2018.
10. Plenary Speaker, "Growth of Metal-Organic Frameworks from Unconventional Precursors," The 13<sup>th</sup> International Conference on the Fundamentals of Adsorption, Cairns, Australia, May 26-31, 2019.

**D2. Invited Conference and Workshop Presentations**

11. "Metal-Organic Frameworks for Adsorption Applications," Workshop on Porous Carbons: Adsorbent Materials for Chemical/Biological Protection, Seattle, WA, July 13-14, 2007.
12. "Challenges and New Directions in Nanostructured Porous Materials Research," Multidisciplinary University Research Initiative Workshop, Arlington, VA, September 3-4, 2007.
13. "Perspectives and Challenges in Adsorption Science and Nanoporous Materials," AIChE/ACS Joint Symposium: Thermodynamics in Chemical Engineering: Prospects and Perspectives, in honor of the 100th anniversary of AIChE, Spring Meeting, New Orleans, LA, April 6-10, 2008.
14. Mu, B.; F. Li; J.R. Karra; and K.S. Walton. "Adsorption of Light Gases in Porous Metal-Organic Frameworks," Revolutionary Approaches to Hazard Mitigation, Edinburgh, Scotland, July 29-30, 2008.

15. "Design Strategies for Nanostructured Materials with Advanced Filtration Capabilities," Chemical/Biological Filtration Strategies Working Group, Arlington, VA, September 10-12, 2008.
16. "Nanostructured Inorganic-Organic Hybrids: Engineering a New Class of Porous Materials," Midwest Thermodynamics and Statistical Mechanics Conference, Wayne State University, Detroit, MI, May 20, 2009.
17. Dynamics and Chemistry of Surfaces and Interfaces Basic Research Workshop, Army Research Office, Savannah, GA, 23–25 June 2009.
18. "Adsorption Properties of Porous Inorganic-Organic Hybrids," Gordon Conference in Solid State Chemistry: New Frontiers in Materials Synthesis and Characterization, Magdalen College, Oxford, UK, August 30 - September 4, 2009.
19. Nonproliferation and Arms Control Technology Working Group, Washington, D. C., November 19, 2009.
20. Surface Science Colloquium, Edgewood Chemical Biological Center, Edgewood, MD, December 9, 2009.
21. "Functional Porous Materials for Adsorption Applications," 16<sup>th</sup> German-American Frontiers of Science Symposium, Alexander von Humboldt Foundation and U.S. National Academy of Sciences, Potsdam, Germany, June 2-5, 2010.
22. "Engineering Porous Materials for Air Purification," Chemical/Biological Filtration Strategies Working Group, Arlington, VA, September 1, 2010. "Structural Stability of Metal-Organic Frameworks," 17<sup>th</sup> German-American Frontiers of Science Symposium, Alexander von Humboldt Foundation and U.S. National Academy of Sciences, Irvine, CA, April 8-11, 2011.
23. "Multifunctional Metal-Organic Frameworks: Concepts for Second Skin Technologies", Dynamic Multifunctional Materials for a Second Skin Concept Workshop, Defense Threat Reduction Agency, Natick, MA, August 4-5, 2011.
24. "Development of Mixed-Matrix Hollow Fiber Membranes using MOFs for Carbon Dioxide Capture from Flue Gas," ACS Symposium on Greenhouse Gases, Denver, CO, August 29, 2011.
25. "Design of Metal-Organic Frameworks for Adsorption Separations and Chemical Sensing," 18<sup>th</sup> German-American Frontiers of Science Symposium, Alexander von Humboldt Foundation and U.S. National Academy of Sciences, Potsdam, Germany, May 8-11, 2012.
26. "Toward the Rational Design of Multifunctional Nanomaterials: Synthesis and Characterization of Nanostructured Metal-Organic Frameworks," NSF CBET Grantees Conference, Washington, D.C., June 6-8, 2012.
27. "Identifying Structural Features that Control Stability of MOFs," Metal-Organic Frameworks for Energy Applications, Division of Energy and Fuels, ACS Meeting, Philadelphia, PA, August 19-23, 2012.
28. "Metal-Organic Frameworks for Air Purification," Chem/Bio Filtration Workshop, Arlington, VA, August 28-29, 2012.
29. "MOF/Nanoparticle Composites for Carbon Monoxide Adsorption and Oxidation," ARO Reactive Chemical Systems Workshop, Providence, RI, October 3-4, 2012.
30. Gordon Research Conference on Nanoporous Materials & Their Applications, Holderness School, Holderness, NH, August 11-16, 2013.

31. Seminar, Air Filtration Working Group, Baltimore, MD, October 8, 2013.
32. Invited Lecture, "Effect of Catenation and Basicity of Pillared Ligands on the Water Stability of MOFs," 7<sup>th</sup> International Symposium on Nanoporous Materials, Nigara Falls, Canada, June 24, 2014.
33. Seminar, Air Filtration Working Group, Arlington, VA, October 21-22, 2014.
34. Invited Lecture, "Understanding the Stability of Metal-Organic Frameworks under Humid Conditions," CCR NiChE Workshop, Measurement Needs in the Adsorption Sciences, NIST, Gaithersburg, MD, November 5-6, 2014.
35. Invited Presentation, "Post-synthetic metal insertion in metal-organic frameworks for enhanced ammonia adsorption from air", Telluride Scientific Research Conference on Metal-Organic Frameworks, Telluride, Colorado, June 18, 2015. Invited Award Lecture, Women Chemists Committee Rising Stars Awards Symposium, ACS Spring Meeting, Denver, CO, March 23, 2015.
36. Invited Presentation, "Sizing It Up: The Different Regimes of Carbon Capture," Gordon Research Conference on Carbon Capture, Utilization & Storage, Stonehill College, Easton, MA, May 31 – June 5, 2015.
37. Invited Presentation, "Post-synthetic metal insertion in metal-organic frameworks for enhanced ammonia adsorption from air", Telluride Scientific Research Conference on Metal-Organic Frameworks, Telluride, Colorado, June 18, 2015.
38. Invited Speaker, "Modulating Adsorption and Stability Properties in Pillared Metal-Organic Frameworks," PacifiChem, Honolulu, Hawaii, December 15-20, 2015.
39. Invited Speaker, "The Different Regimes of Carbon Capture: Challenges and Opportunities," Frontiers of Carbon Capture, Utilization, and Storage, 2016 EU-US Frontiers of Engineering Symposium, National Academy of Engineering, Helsinki, Finland, October 16-19, 2016.

### **D3. Conference and Workshop Presentations**

Over 100 presentations at conferences and workshops

### **D4. Invited Seminar Presentations**

1. LeVan, M.D., and K. S. Walton. "Adsorption Research for Space Exploration," seminar given in celebration of 10 years of adsorption research at UFC, Departamento de Engenharia Química, Universidade Federal do Ceará, Fortaleza, Brazil, July 2004.
2. "Novel Nanoporous Materials for Adsorption Applications," Chevron Phillips, CPChem, Bartlesville, OK, September 25, 2007.
3. Seminar, Department of Chemical Engineering, University of Edinburgh, Edinburgh, Scotland, U.K., August 1, 2008.
4. Seminar, Department of Chemical Engineering, University of Virginia, Charlottesville, VA, October 16, 2008.
5. Seminar, Department of Chemical Engineering, Arizona State University, Tempe, AZ, October 31, 2008.

6. Seminar, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, January 7, 2009.
7. Seminar, Department of Chemical Engineering, West Virginia University, October 30, 2009.
8. Seminar, Department of Chemical Engineering, University of Washington, Seattle, WA, January 10, 2011.
9. Seminar, Adsorption Research Group, Air Products & Chemicals, Allentown, PA, January 19, 2011.
10. Seminar, Quantachrome Instruments, Boynton Beach, FL, February 21, 2011.
11. Seminar, Department of Chemistry, University of California-Berkeley, September 30, 2011.
12. Seminar, Department of Chemical Engineering, University of Arkansas, October 4, 2011.
13. Seminar, Department of Chemical and Biomolecular Engineering, Vanderbilt University, Feb 20, 2012.
14. Seminar, Adsorption Research Group, Quantachrome Instruments, Boynton Beach, FL, March 21, 2012
15. Seminar, Department of Chemistry, University of South Florida, October 11, 2012.
16. Seminar, Department of Chemistry, University of Vermont, November 29, 2012.
17. Seminar, Department of Chemical Engineering, University of Florida, March 11, 2013.
18. Seminar, ExxonMobil Research and Engineering, Clinton, NJ, November 12, 2013.
19. Seminar, Eastman Chemical, Kingsport, TN, November 19, 2013.
20. Seminar, Department of Chemistry, University at Buffalo, Buffalo, NY, April 18, 2014
21. Seminar, Department of Chemical Engineering, University of Missouri, September 22, 2015.
22. Seminar, School for Engineering of Matter, Transport, and Energy, Arizona State University, February 22, 2016.
23. Seminar, Department of Chemical and Biological Engineering, Princeton University, March 30, 2016.
24. Seminar, University of Amsterdam, April 29, 2016.
25. Seminar, Filtration and Separation Chapter, 3M Center, St. Paul, MN, July 14, 2016
26. Seminar, Department of Chemical Engineering, Penn State University, September 29, 2016
27. Seminar, Department of Chemistry, Virginia Tech, February 10, 2017.
28. Seminar, Department of Chemistry, University of Delaware, November 17, 2017
29. Seminar, Department of Mechanical and Process Engineering, ETH Zurich, Switzerland, November 4, 2018.
30. Seminar, Department of Chemical Engineering, University of Massachusetts Amherst, March 5, 2019.
31. Seminar, Department of Chemical & Biomolecular Engineering, University of Houston, October 18, 2019.

**E. GRANTS AND CONTRACTS (Total external funding raised as PI since 2006: \$31M)**

- Professor Walton has raised \$31 million in external funds from federal agencies and industry
- Research sponsors and collaborators include, Army Research Office, Defense Threat Reduction Agency, Department of Defense, Department of Energy, ARPA-E, Dow, ExxonMobil, NASA, National Science Foundation, Praxair, United Technologies

**F. OTHER SCHOLARLY AND CREATIVE ACCOMPLISHMENTS**

- Co-Founder, Inmondo Tech, Inc., 2013
- Co-Founder, Ipsum Nano, LLC, 2016

**G. SOCIETAL AND POLICY IMPACTS**

The aim of my research is to advance the state-of-the-art in porous materials by uncovering structure-property relationships that will lead to commercialization of new classes of materials for air purification, carbon dioxide capture, and other chemical separations that are important to the environment.

**H. OTHER PROFESSIONAL ACTIVITIES**

Consulting

- United Technologies Research Corporation, May 2009 – July 2009
- Illinois Tool Works, March 2011 – 2013
- Eprida, Inc, January 2012-2013
- Barnes & Thornburg, November 2017 – present

**V. TEACHING****A. INDIVIDUAL STUDENT GUIDANCE****A1. Ph.D. Students****A1.a. Graduated**

1. Bin Mu, Ph.D. 2011, "Synthesis and Gas Adsorption Study of Porous Metal-Organic Framework Materials," Current Position: Assistant Professor, Arizona State University.
2. J. Reddy Karra, Ph.D. 2011, "Development of Porous Metal Organic Frameworks for Gas Adsorption Applications," Current Position: Research Engineer, UTRC.
3. Paul Schoenecker, Ph.D. 2012, "High-Throughput Synthesis and Application of Water-Stable MOFs," Current Position: Research Engineer, Air Products
4. Yang Cai, Ph.D. 2013, "Impact of Ligand Functionalization on 1,3,5-Benzene Tricarboxylic Acid MOFs."
5. Katrina Stults, Ph.D. 2014, "Metal Oxide-MOF Composites for Toxic Gas Removal from Air," Current Position: Analytical Services Manager, Quantachrome Instruments.
6. Greg Cmarik, Ph.D. 2014, "Application of Post-Synthetic Modification to Metal-Organic Frameworks to Develop Water-Resistant, High Efficiency Adsorbents for Carbon Dioxide Separations."
7. Himanshu Jasuja, Ph.D. 2014, "Developing Design Criteria and Scale Up Methods for Water-Stable Metal-Organic Frameworks for Adsorption Applications," Current Position: Senior Product Development Engineer, 3M.
8. Michael Mangarella, Ph.D. 2015, "Synthesis and Characterization of Carbide Derived Carbons for Selective Adsorption of Toxic Gases."

9. Nicholas Burtch, Ph.D. 2016, "A Priori Identification of Water Stable Metal-Organic Frameworks for Selective Gas Adsorption and Air Purification Applications." Current Position: Truman Fellow, Sandia National Lab
10. Karen Tulig, Ph.D. 2016, "Synthesis and Application of Metal-Organic Framework/Metal Nanoparticle Composites." Current Position: Senior Engineer, Intel
11. William Mounfield, Ph.D. 2016, "Metal-Organic Frameworks for CO<sub>2</sub> Capture." Current Position: Postdoctoral Associate at MIT.
12. Michael Dutzer, Ph.D. 2017, "Low-Cost Carbide-Derived Carbons for Adsorptive Removal of VOCs from Air Streams." Current Position: Senior Process Engineer, Intel.
13. Yang Jiao, Ph.D. 2017, "Novel MOF/Nanoparticle Architectures for Catalytic Applications." Current Position: Senior Research Engineer, Intel.
14. Lalit Darunte, Ph.D. 2018, "Supported Amines in Metal-Organic Frameworks for Air Capture." Co-advised with Prof. Christopher Jones and Prof. David Sholl. Current Position: Senior Engineer, Dow.
15. Colton Moran, Ph.D. 2018, "Design and Application of Carbide-Derived Carbons." Current Position: Associate, Exponent.
16. Jacob Deneff, Matriculation Fall 2014, Ph.D. Candidate, "MOF Composites for Removal and Sensing of Chemical Warfare Agents."
17. Julian Hungerford, Matriculation Fall 2014, Ph.D. Candidate, "Mixed Metal MOFs for Acid Gas Removal."
18. Jayraj Joshi, Matriculation Fall 2014, Ph.D. Candidate, "Enhancement of Sour Gas Removal through Tuning the Chemical Properties of Metal-Organic Frameworks."

#### **A.1.b. In Process**

19. Eli Carter, Matriculation Fall 2015, Ph.D. Candidate, "Multicomponent Adsorption and Acid Gas Effects in Metal-Organic Frameworks."
20. Yutao Gong, Matriculation Fall 2015, Ph.D. Candidate, "Tuning Adsorption Interactions of Metal-Organic Frameworks for Ethylene and Ethane Separation."
21. Carmen Chen, PhD Candidate.
22. Brandon Bout, Matriculation Fall 2017.
23. Daniel Shade, PhD Candidate.
24. Rohan Murty, Matriculation Fall 2017, co-advised with Prof. Mark Prausnitz.
25. Tania Evans, Matriculation Fall 2018.
26. Chengzhai Wang, Matriculation Fall 2018.
27. Lukas Bingel, Matriculation Fall 2019.
28. Lape Oghenetega, Matriculation Fall 2019.

#### **A2. M.S. Students**

##### **B.2.a. Graduated with M.S. Thesis**

1. Christine Flemming, M.S. 2012, "Synthesis and Characterization of Metal-Organic Frameworks as Base Catalysts," Current Position: Process Engineer, Cummins, Inc.
2. Ken Onubogu, M.S. 2014, "Effect of Binder Amount and Calcination Temperature on the Physical and Mechanical Properties of Pressed Metal-Organic Framework UiO-66." Co-advised with Prof. David Sholl. Current Position: Process Engineer, MeadWestvaco
3. Erika Garcia-Gutierrez, M.S. 2015, "Copper Insertion in a Series of Metal-Organic Frameworks with Uncoordinated Carboxylic Acid Groups for Ammonia Removal," Current Position: Process Engineer, HP.

4. Jayraj Joshi, M.S. 2016, "Copper Insertion in UiO-66 Analogues for Ammonia Removal Applications," Current Position: PhD Student at Georgia Tech

### **A.3. Undergraduate Students**

#### **Georgia Tech:**

1. Joshua Cruz, Spring 2010
2. Thomas Devine, Spring 2010
3. Chien Wei Wang, Fall 2010 (*Co-Advised with David Sholl and Sankar Nair*)
4. Victor Manrique, Fall 2010-Spring 2011 (*Co-Advised with David Sholl and Sankar Nair*)
5. Megan DeWitt, Fall 2010-Spring 2011 (*Co-Advised with David Sholl and Sankar Nair*)
6. Stella Kinnaird, Fall 2010-Spring 2011 (*Co-Advised with David Sholl and Sankar Nair*)
7. Madison Barre, Fall 2010-Spring 2011 (*Co-Advised with David Sholl and Sankar Nair*)
8. Chris Kim, Fall 2010-Spring 2011 (*Co-Advised with David Sholl and Sankar Nair*)
9. Grace Belancik, Spring-Summer 2011 (PURA winner for Summer 2011)
10. Arthur Barfield, Summer 2011
11. Deonte Fletcher, Spring/Summer/Fall 2012
12. Thomas Brumby, Fall 2012/Spring 2013
13. Pooja Sujit, Fall 2012/Spring 2013
14. Jacob Harris, Fall 2013/Spring 2014
15. Luiz Nunez, Fall 2013/Spring 2014
16. Myles Everett, Spring 2015
17. Davin Oetomo, Spring 2015 – Spring 2017
18. Maya Barroso, Spring/Fall 2016
19. Stephanie Varughese, Fall 2016/Spring 2017
20. James Dow, Fall 2017/Spring 2018
21. Harold Feininger, Spring 2018/Summer 2018
22. Zachery Flowers, Spring 2018/Fall 2018

#### **Kansas State University:**

1. Jordon Groskurth, Spring 2008 – Spring 2009
2. Levi Naden, Summer 2008
3. Jason Orr, Summer-Fall 2008
4. Zachary Farrell, Fall 2008

### **A.4. Mentorship of Postdoctoral Fellows**

1. Dr. Bartosz Marsalek, 2018-current
2. Dr. Xiao Jiang, 2017-current
3. Dr. Ian Walton, 2016-current
4. Dr. Ross Verplough, 2017-2018
5. Dr. Michael Mangarella, 2016
6. Dr. Sudhir Sharma, 2016
7. Dr. Yi Harvey Huang, 2015-2017
8. Dr. Bogna Grabicka, 2011-2016
9. Dr. Cody Morelock, 2014-2016
10. Dr. Christopher Murdock, 2014-2016, co-advised with C. Jones
11. Dr. Tim Duerinck, 2014-2015
12. Dr. Yougui Huang, 2008-2013



13. Dr. Sangil Han, 2010-2012, Co-Advised with D. Sholl, C. Meredith, S. Nair, C. Jones, W. Koros
14. Dr. Taku Watanabe, 2010-2012, Co-Advised with D. Sholl, S. Nair, C. Meredith, C. Jones, W. Koros
15. Dr. Ying Dai, 2010-2012, Co-Advised with W. Koros, D. Sholl, S. Nair C. Meredith, C. Jones
16. Dr. Cantwell Carson, 2009-2011
17. Dr. Feng Li, 2007-2008

## **B. COURSE DEVELOPMENT**

Created an elective on advanced separations (ChBE 4803/6240) that is cross-listed for graduate students and upper-level undergraduates. Spring 2019 was the first offering of the course.

## **VI. SERVICE**

### **A. PROFESSIONAL CONTRIBUTIONS**

#### **A1. Editorial Board Memberships**

- Board of Directors, International Adsorption Society, 2010-2015
- Editorial Board, *Adsorption Journal*, 2013-2015
- Editorial Board, *Separation Science and Technology*, 2012-2014

#### **A2. Society Offices, Activities, and Membership**

- Secretary/Treasurer, International Adsorption Society, 2010-2015
- MOF Council to the International Zeolite Association, North America Representative, 2012-present
- Director, Separations Division, American Institute of Chemical Engineers, 2008-2014
- Chair, AIChE Separations Division Area 2e, 2013-2015
- Vice-Chair, AIChE Separations Division Area 2e Adsorption and Ion Exchange, 2011-2013
- American Chemical Society, member since 2007

#### **A3. Organization and Chairmanship of Technical Sessions, Workshops, and Conferences**

- Co-Chair, 14<sup>th</sup> International Conference on Fundamentals of Adsorption (FOA14), 2022.
- Organizing Committee of Separations Technology IX: New Frontiers in Media, Technique, and Technologies, March 2017.
- Organizing Committee of the 5<sup>th</sup> International Conference on Metal-Organic Frameworks & Open Framework Compounds, October 2016
- German-American Frontiers of Science, U.S. National Academies and Alexander von Humboldt Foundation: Participant (2010); Organizing committee (2011); Meeting Chair, U.S., (2012)
- Programming Committee member, AIChE Area 2e Adsorption and Ion Exchange, 2006- present
- Session Chair, Area 2e AIChE Annual Meeting, > 20 sessions since 2006
- Study Committee member, National Research Council, Examining Activated Carbon Disposal at U.S. Army Chemical Demilitarization Sites, 2008-2009
- Panelist for Chemical Safety Summit organized by the National Academies Board on Chemical Sciences & Technology, Washington, D.C., November 2010.

**A4. Technical Journal or Conference Referee Activities**

- Associate Editor, Industrial & Engineering Chemistry Research, 2014-present
- > 200 articles reviewed since 2006  
Adsorption, Adsorption Science and Technology, Advanced Functional Materials, Advanced Materials, Angewandte Chemie International Edition, Applied Surface Science, Chemical Engineering Science, Chemical Communications, Chemical Reviews, Chemistry of Materials, ChemPhysChem, ChemSusChem, CrystEngComm, Crystal Growth & Design, Energy & Environmental Science, Energy and Fuels, Fluid Phase Equilibria, Industrial & Engineering Chemistry Research, Inorganic Chemistry, Journal of the American Chemical Society, Journal of Materials Chemistry, Journal of Membrane Science, Nature Communications, Journal of Physical Chemistry C, Langmuir, Molecular Physics, Molecular Simulation, Nature Chemistry, Physical Chemistry Chemical Physics, Proceedings of the National Academy of Sciences, Sensors & Actuators

**A5. Proposal Panels and Reviews**

1. National Science Foundation, review panels: 25+ panels since 2007
2. Defense Threat Reduction Agency, review panel, 2008
3. American Chemical Society Petroleum Research Fund, mail reviewer: 6 since 2006
4. DoD, Army Research Office, Mail Reviewer: >20 since 2007
5. Kentucky Science and Engineering Foundation R&D Excellence Award, mail reviewer, 2011
6. US Civilian Research & Development Foundation, mail reviewer, 2011

**A6. Other Involvement**

- US Representative, Global Young Academy, 2012-2016

**B. PUBLIC AND COMMUNITY SERVICE**

- Hosted chemistry teacher from local high school in the lab in summer 2010 for GIFT program, along with her three high school students. Their project centered on identifying reaction conditions to control the size and rate of crystal formation in MOF synthesis
- Mentor, female high school student (rising junior) summer research experience, 2011
- Mentor for underrepresented minority undergraduate student through the Georgia Tech PURA program, summer 2018

**C. INSTITUTE CONTRIBUTIONS****C1. Institute Committee Service:**

- COE Representative to the Strategic Plan Advisory Group, 2017-2019
- COE Representative, College of Sciences Dean Search, 2018-2019
- Search Committee, Research Development Specialist for the new Grants Hatchery, 2019

**C2. College Committee Service**

- College of Engineering Reappointment, Promotion, and Tenure Committee, 2012-2014; 2017-2019
- College of Engineering Strategic Planning Committee, 2018-2019

**C3. School Committee Service**

- ChBE Faculty Search Committee, 2012-2013; 2016-present
- ChBE Seminar Committee, 2012-2014
- ChBE Graduate Studies Committee, 2012-2018
- ChBE School Chair Search Committee, 2012-2013
- ChBE Newsletter committee, 2009-2012
- ChBE Representative, GT Academic Senate and General Faculty Assembly
- ChBE 4<sup>th</sup> Year Colloquium, 2013, Organizer