

Curriculum Vitae – David S. Sholl

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Education

Ph.D., University of Colorado, Program in Applied Mathematics, Boulder, CO, 1995.
(Advisor: Prof. Rex T. Skodje, Dept. of Chemistry)
M.Sc., University of Colorado, Program in Applied Mathematics, Boulder, CO, 1993.
B.Sc. (with Honors and University Medal), Theoretical Physics,
The Australian National University, Canberra, ACT, Australia, 1992.

Employment

10/16 - , John F. Brock III School Chair, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA
7/13 – 9/16 , School Chair, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA
1/08 – 9/16, Michael E. Tennenbaum Family Chair and GRA Eminent Scholar in Energy Sustainability, School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA
1/10-6/13 , Associate Director, Strategic Energy Institute, Georgia Institute of Technology, Atlanta, GA
7/06-12/07 , Professor, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA
7/02 –6/06 , Associate Professor, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA
8/03 – 12/07, Courtesy Faculty, Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA
1/98 – 6/02, Assistant Professor, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA.
2/97-12/97, Postdoctoral researcher, Department of Chemistry, Yale University, New Haven, CT. (Advisor: Prof. John C. Tully)
2/96-2/97, Postdoctoral researcher, Departments of Chemical Engineering and Physics, The Pennsylvania State University, State College, PA. (Advisor: Prof. Kristen A. Fichthorn)

Leadership Roles

1. Board of Directors, American Institute of Chemical Engineers, 2019-2021
2. Chair, Inaugural Gordon Conference on Chemical Separations, 2020
3. Organizing Committee Member, Inaugural Chemical Engineering National Diversity Equity Workshop, 2019-2020

4. Panel member, National Academies Study Committee, Research Agenda for a New Era in Separations Science, 2018-2019
5. Member, AIChE Strategic Plan Steering Committee, 2018
6. Interim Chief Technology Officer (8/16-3/17) and Focus Area Lead (Modeling & Simulation) (3/17-present), RAPID National Manufacturing Institute, AIChE.
7. Co-chair, DOE BES Basic Research Needs Workshop on the Energy-Water Nexus, 2017.
8. School Chair, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, 7/13-present.
9. Co-chair, International Conference on Inorganic Membranes 2016.
10. Chair, Gordon Conference on Nanoporous Materials, 8/15.
11. Deputy Director, UNCAGE-ME (DOE Energy Frontier Research Center), 8/14-present.
12. Chair, Computational Molecular Science and Engineering Forum, AIChE, 2012-2014.
13. Co-founder, *InmondoTech Inc.*, 2013-2018
14. Associate Director, Strategic Energy Institute, Georgia Institute of Technology, Atlanta, GA, 1/10-6/13.
15. Senior editor, *Langmuir*, 2009-present.

Awards and Distinctions

1. Inaugural Ma Lecturer, Department of Chemical Engineering, Worcester Polytechnic Institute (2019)
2. Institute Award for Excellence in Industrial Gases Technology, American Institute of Chemical Engineering (2018)
3. Parr Lecturer, Department of Chemical and Biomolecular Engineering, University of Illinois (2018)
4. “Highly Prolific Author” recognition, *Journal of Physical Chemistry C* (2017)
5. AIChE Gary Leach Award [jointly with several faculty and staff from Georgia Tech] (2015)
6. Early Career Achievement Award, Computational Molecular Science and Engineering Forum, AIChE (2010)
7. DOE Hydrogen Program R&D Award (2008)
8. MESD Plenary Session speaker, AIChE Annual Meeting (2007)
9. COMSEF Plenary Session speaker, AIChE Annual Meeting (2006)
10. CAST Plenary Session speaker, AIChE Annual Meeting (2002)
11. Camille Dreyfus Teacher-Scholar Award (2002)
12. E. Kears Pollock/PPG Industries Grant for Young Faculty (2002-2005)
13. Alfred P. Sloan fellow (2001-2003)
14. George Tallman Ladd Award for Excellence in Research, Carnegie Institute of Technology, Carnegie Mellon University (2000)
15. National Science Foundation CAREER Award (2000-2004)
16. Faculty Fellow, National Energy Technology Laboratory (2000-2007)
17. APS Division of Chemical Physics Travel Award (1996).
18. University of Colorado Graduate School Research and Creative Work Award (1995).
19. Honorable mention, NSF Graduate Research Fellowship (1991).

20. University of Colorado Doctoral Fellowship (1991).
21. University Medal, Australian National University (1991).
22. Education Abroad Scholar, University of California (1988-1989).
23. National Undergraduate Scholarship, Australian National University (1987-1991).

Research Publications (> 15,700 citations, h-index = 69 as reported by Web of Science)
[Publications with > 50 citations indicated by * and with > 100 citations indicated by **]

1. *Predictions of Hg⁰ and HgCl₂ adsorption properties in UiO-66 from flue gas using molecular simulations*, Hongjian Tang, Hanjun Fang, Yufeng Duan and David S. Sholl, *Journal of Physical Chemistry C*, 123 (2019) 5972-5979
2. *Stability of zeolitic imidazolate frameworks in NO₂*, Sourydeep Bhattacharyya, Rebecca Han, Jayraj N. Joshi, Guanghui Zhu, Ryan P. Lively, Krista S. Walton, David S. Sholl, Sankar Nair, *Journal of Physical Chemistry C*, 123 (2019) 2336-2346
3. *In silico prediction of structural properties of a racemic porous organic crystal*, Yang Liu, Guanghui Zhu, Wenqin You, Hongjian Tang, Christopher W. Jones, Ryan P. Lively and David S. Sholl, *Journal of Physical Chemistry C*, 123 (2019) 1720-1729
4. *A database of computation-ready 2D zeolitic slabs*, Omar Knio, Andrew J. Medford, Sankar Nair and David S. Sholl, *Chemistry of Materials*, 31 (2019) 353-364
5. *Moving beyond adsorption capacity in design of adsorbents for CO₂ capture from ultradilute feeds: Kinetics of CO₂ adsorption in materials with stepped isotherms*, Lalit A. Darunte, Trisha Sen, Chiraag Bhawanani, Krista S. Walton, David S. Sholl, Matthew J. Realff, and Christopher W. Jones, *Industrial & Engineering Chemistry Research*, 58 (2019) 366-377
6. *Tuning binding tendencies of small molecules in metal-organic frameworks with open metal sites by metal substitution and linker functionalization*, Wenqin You, Yang Liu, Joshua D. Howe, Dai Tang and David S. Sholl, *Journal of Physical Chemistry C*, 122 (2018) 27486-27494
7. *How useful are common simulants of chemical warfare agents at predicting adsorption behavior?*, Mayank Agrawal, Dorina F. Sava Gallis, Jeffery A. Greathouse and David S. Sholl, *Journal of Physical Chemistry C*, 122 (2018) 26061-26069
8. *Molecular simulation of capture of sulfur-containing gases by porous aromatic frameworks*, Difan Zhang, Xiaofei Jing, David S. Sholl and Susan B. Sinnott, *Journal of Physical Chemistry C*, 122 (2018) 18456-18467
9. *Assessing the impact of point defects on molecular diffusion in ZIF-8 using molecular simulations*, Chu Han, Ross J. Verploegh and David S. Sholl, *Journal of Physical Chemistry Letters*, 9 (2018) 4037-4044
10. *Acid gas stability of zeolitic imidazolate-frameworks: Generalized kinetic and thermodynamic aspects*, Souryadeep Bhattacharyya, Rebecca Han, Wun-Gwi Kim, Yadong Chiang, Krishna C. Jayachandrababu, Julian T. Hungerford, Michael R. Dutzer, Chen Ma, Krista S. Walton, David S. Sholl and Sankar Nair, *Chemistry of Materials*, 30 (2018) 4089-4101
11. *First-principles-derived force fields for CH₄ adsorption and diffusion in siliceous zeolites*, Hanjun Fang, Rohan Awati, Salah E. Boulfefel, Peter I Ravikovitch, and David S. Sholl, *Journal of Physical Chemistry C*, 122 (2018) 12880-12891

12. *The effect of aluminum short-range ordering on carbon dioxide adsorption in zeolites*, John M. Findley, Peter I. Ravikovitch and David S. Sholl, *Journal of Physical Chemistry C*, 122 (2018) 12332-12340
13. *Efficiently exploring adsorption space to identify privileged adsorbents for chemical separations of a diverse set of molecules*, Dai Tang, Ying Wu, Ross J. Verploegh and David S. Sholl, *ChemSusChem*, 11 (2018) 1567-1575
14. *Competitive binding of ethylene, water, and carbon monoxide in metal-organic framework materials with open Cu sites*, Wenqin You, Yang Liu, Joshua D. Howe and David S. Sholl, *Journal of Physical Chemistry C*, 122 (2018) 8960-8966
15. *Quantitative predictions of molecular diffusion in binary mixed-linker zeolitic imidazolate frameworks using molecular simulation*, Ross J. Verploegh, Ying Wu, Salah Eddine Boulfefel and David S. Sholl, *Journal of Physical Chemistry C*, 122 (2018) 5627-5638
16. *Insights into the stability of zeolitic imidazolate frameworks in humid acidic environments from first-principles calculations*, Chu Han, Chenyang Zhang, Nina Tyminska, J. R. Schmidt and David S. Sholl, *Journal of Physical Chemistry C*, 122 (2018) 4339-4348
17. *Writing theory and modeling papers for Langmuir: The good, the bad and the ugly (Editorial)*, Han Zuilhof, Shu-Hong Yu and David S. Sholl, *Langmuir* 34 (2018) 1817-1818
18. *Liquid-phase multicomponent adsorption and separation of xylene mixtures by flexible MIL-53 adsorbents*, Mayank Agrawal, Souryadeep Bhattacharyya, Yi Huang, Krishna C. Jayachandrababu, Christopher R. Murdock, Jason A. Bentley, Alejandra Rivas-Cardona, Machteld M. Mertens, Krista S. Walton, David S. Sholl and Sankar Nair, *Journal of Physical Chemistry C*, 122 (2018) 386-397
19. *Formation mechanisms and defect engineering of imine-based porous organic cages*, Guanghui Zhu, Yang Liu, Luis Flores, Zachary R. Lee, Christopher W. Jones, David A. Dixon, David S. Sholl and Ryan P. Lively, *Chemistry of Materials*, 30 (2018) 262-272
20. *How reproducible are isotherm measurements in metal-organic frameworks?* Jongwoo Park, Joshua D. Howe and David S. Sholl, *Chemistry of Materials*, 29 (2017) 10487-10495
21. *CO₂ dynamics in pure and mixed-metal MOFs with open metal sites*, Robert M. Marti, Joshua D. Howe, Cody R. Morelock, Mark S. Conradi, Krista S. Walton, David S. Sholl and Sophia E. Hayes, *Journal of Physical Chemistry C*, 121 (2017) 25778-25787
22. *Research challenges in avoiding “showstoppers” in developing materials for large-scale energy applications*, Krista S. Walton and David S. Sholl, *Joule*, 1 (2017) 208-211
23. *Heat-treatment of defective UiO-66 from modulated synthesis: Adsorption and stability studies*, Yang Jiao, Yang Liu, Guanghui Zhu, Julian T. Hungerford, Souryadeep Bhattacharyya, Ryan P. Lively, David S. Sholl and Krista S. Walton, *Journal of Physical Chemistry C*, 121 (2017) 23471-23479
24. *Recovery of acid-gas-degraded zeolitic imidazolate frameworks by solvent-assisted crystal redemption (SACRed)*, Krishna C. Jayachandrababu, Souryadeep

- Bhattacharyya, Yadong Chiang, David S. Sholl and Sankar Nair, ACS Applied Materials and Interfaces, 9 (2017) 34597-34602
25. *Computational screening of functionalized UiO-66 materials for selective contaminant removal from air*, Hakan Demir, Krista S. Walton and David S. Sholl, Journal of Physical Chemistry C, 121 (2017) 20396-20406
 26. *Effect of surface structure of TiO₂ nanoparticles on CO₂ adsorption and SO₂ resistance*, Uma Tumuluri, Joshua D. Howe, William P. Mounfield, Meijun Li, Miaofang Chi, Zachary D. Hood, Krista S. Walton, David S. Sholl, Sheng Dai and Zili Wu, ACS Sustainable Chemistry & Engineering, 5 (2017) 9295-9306
 27. *Butanol separation from humid CO₂-containing multicomponent vapor mixtures by zeolitic imidazolate frameworks*, Souryadeep Bhattacharyya, Krishna C. Jayachandrababu, Yadong Chiang, David S. Sholl and Sankar Nair, ACS Sustainable Chemistry & Engineering, 5 (2017) 9467-9476
 28. *Modeling and process simulation of hollow fiber membrane reactor systems for propane dehydrogenation*, Seung-Won Choi, David S. Sholl, Sankar Nair, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, John G. Prendergast, AIChE Journal 63 (2017) 4519-4531
 29. *Hierarchical Ga-MFI catalysts for propane dehydrogenation*, Wun-gwi Kim, Jungseob So, Seung-Won Choi, Yujun Liu, Ravindra S. Dixit, Carsten Sievers, David S. Sholl, Sankar Nair and Christopher W. Jones, Chemistry of Materials, 29 (2017) 7213-7322
 30. *Towards the directional transport of molecules on surfaces*, Natalie A. Wasio, Colin J. Murphy, Dipna A. Patel, Daniel Wei, David S. Sholl and E. Charles H. Sykes, Tetrahedron, 73 (2017) 4858-4863
 31. *Impacts of gas impurities from pipeline natural gas on methane storage in metal-organic frameworks during long-term cycling*, Ying Wu, Dai Tang, Ross J. Verploegh, Hongxia Xi and David S. Sholl, Journal of Physical Chemistry C, 121 (2017) 15735-15745
 32. *Lattice-gas modeling of adsorbate diffusion in mixed-linker zeolitic imidazolate frameworks: Effect of local imidazolate ordering*, Ross J. Verploegh, Ying Wu and David S. Sholl, Langmuir, 33 (2017) 6481-6491
 33. *First-principles investigation of chemical stability and proton conductivity in M-doped BaZrO₃ (M = K, Rb, and Cs)*, Journal of the American Ceramic Society, 100 (2017) 2997-3003
 34. *Establishing upper bounds on CO₂ swing capacity in sub-ambient pressure swing adsorption via molecular simulation of metal-organic frameworks*, Jongwoo Park, Ryan P. Lively and David S. Sholl, Journal of Materials Chemistry A, 5 (2017) 12258-12265
 35. *Temperature-regulated guest admission and release in microporous materials*, Gang Li, Jin Shang, Qinfen Gu, Rohan V. Awati, Nathan Jensen, Andrew Grant, Xueying Zhang, David S. Sholl, Jefferson Z. Liu, Paul A. Webley and Eric F. May, Nature Communications, 8 (2017) 15777
 36. *Monolith-supported amine-functionalized Mg₂(dobpdc) adsorbents for CO₂ capture*, Lalit A. Darunte, Yuri Terada, Christopher R. Murdock, Krista S. Walton, David S. Sholl, and Christopher W. Jones, ACS Applied Materials and Interfaces, 9 (2017) 17043-17051

37. *Structural and mechanistic differences in mixed-linker zeolitic imidazolate framework synthesis by solvent assisted linker exchange and de novo routes*, Krishna C. Jayachandrababu, David S. Sholl and Sankar Nair, *Journal of the American Chemical Society*, 139 (2017) 5906-5915
38. *Acid gas adsorption on metal-organic framework nanosheets as a model of an “all-surface” material*, Joshua D. Howe, Yang Liu, Luis Flores, David A. Dixon and David S. Sholl, *Journal of Chemical Theory and Computation*, 13 (2017) 1341-1350
39. *From water to organics in membrane separations*, Ryan P. Lively and David S. Sholl, *Nature Materials* 16 (2017) 276-279
40. *Understanding structure, metal distribution, and water adsorption in mixed-metal MOF-74*, Joshua D. Howe, Cody R. Morelock, Yang Jiao, Karena W. Chapman, Krista S. Walton and David S. Sholl, *Journal of Physical Chemistry C*, 121 (2017) 627-635
41. *Large-scale refinement of metal organic framework structures using DFT*, Chemistry of Materials, Dalar Nazarian, Jeffrey S. Camp, Yongchul G. Chung, Randall Q. Snurr and David S. Sholl, *Chemistry of Materials*, 29 (2017) 2521-2528
42. *Computational investigation on CO₂ adsorption in titanium carbide-derived carbons with residual titanium*, Difan Zhang, Michael R. Dutzer, Tao Liang, Alexandre F. Fonseca, Ying Wu, Krista S. Walton, David S. Sholl, Amir H. Farmahini, Suresh K. Sinnott, and Susan B. Sinnott, *Carbon*, 111 (2017) 741-751
43. *Characterizing chemical stability and proton conductivity of B-site doped barium hafnate (BaHfO₃) and barium stannate (BaSnO₃) with first principles modeling*, Sung Gu Kang and David S. Sholl, *Journal of Alloys and Compounds*, 693 (2017) 738-743
44. *Propane dehydrogenation catalyzed by gallosilicate MFI zeolites with perturbed acidity*, Seung-Won Choi, Wun-Gwi Kim Jung-Seob So, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, John G. Pendergast, Carsten Sievers, David S. Sholl, Sankar Nair, and Christopher W. Jones, *Journal of Catalysis*, 345 (2017) 113-123
45. *Computational model and characterization of stacking faults in ZIF-8 polymorphs*, Rebecca Han and David S. Sholl, *Journal of Physical Chemistry C*, 120 (2016) 27380-27388
46. *Interactions of SO₂-containing acid gases with ZIF-8: Structural changes and mechanistic investigations*, Souryadeep Bhattacharyya, Simon H. Pang, Michael R. Dutzer, Ryan P. Lively, Krista S. Walton, David S. Sholl and Sankar Nair, *Journal of Physical Chemistry C*, 120 (2016) 27221-27229
47. *Synergistic effects of water and SO₂ on degradation of MIL-125 in the presence of acid gases*, William P. Mounfield III, Chu Han, Simon H. Pang, Uma Tumuluri, Yang Jiao, Souryadeep Bhattacharyya, Michael R. Dutzer, Sankar Nair, Zili Wu, David S. Sholl and Krista S. Walton, *Journal of Physical Chemistry C*, 120 (2016) 27230-27240
48. *Screening of copper open metal site MOFs for olefin/paraffin separations using DFT-derived force fields*, Ambarish Kulkarni and David S. Sholl, *Journal of Physical Chemistry C*, 120 (2016) 23044-23054
49. *Facet-specific stability of ZIF-8 in the presence of acid gases dissolved in aqueous solution*, Simon H. Pang, Chu Han, David S. Sholl, Christopher W. Jones, and Ryan P. Lively, *Chemistry of Materials*, 28 (2016) 6960-6967

50. *One-Step Synthesis of Zeolite Membranes Containing Catalytic Metal Clusters*, Seok-Jhin Kim, Shuai Tan, Micaela Taborga Claire, Laura Gil Briones, Karren L. More, Yujun Liu, Jason S. Moore, Ravindra S. Dixit, John G. Pendergast, David S. Sholl, Christopher W. Jones and Sankar Nair, *ACS Applied Materials and Interfaces*, 37 (2016) 24671-24681
51. *Propane dehydrogenation over alumina-supported iron/phosphorous catalysts: Structural evolution of iron species leading to high activity and propylene selectivity*, Shuai Tan, Bo Hu, Wun-Gwi Kim, Simon H. Pang, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, John G. Pendergast, David S. Sholl, Sankar Nair, Christopher W. Jones, *ACS Catalysis*, 6 (2016) 5673-5683
52. *Engineering porous organic cage crystals with increased acid gas resistance*, Guanghui Zhu, Christopher D. Hoffman, Yang Liu, Souryadeep Bhattacharyya, Uma Tumuluri, Melinda L. Jue, Zili Wu, David S. Sholl, Sankar Nair, Christopher W. Jones, Ryan P. Lively, *Chemistry European Journal*, 22 (2016) 10743-10747
53. *Improved Hill-Sauer force field for accurate description of pores in 8-ring zeolites*, Salah Eddine Boulfefel, Peter I. Ravikovitch, Lucas Koziol, and David S. Sholl, *Journal of Physical Chemistry C*, 120 (2016) 14140-14148
54. *CO₂ capture via adsorption in amine-functionalized sorbents*, Lalit A. Darunte, Krista S. Walton, David S. Sholl and Christopher W. Jones, *Current Opinion in Chemical Engineering*, 12 (2016) 82-90
55. *Structure elucidation of mixed-linker zeolitic imidazolate frameworks by solid-state ¹H CRAMPS NMR spectroscopy and modeling*, Krishna C. Jayachandrababu, Ross J. Verploegh, J. Leisen, Ryan C. Nieuwendaal, David S. Sholl and Sankar Nair, *Journal of the American Chemical Society*, 138 (2016) 7325-7336
56. *Thin hydrogen-selective SAPO-34 zeolite membranes for enhanced conversion and selectivity in propane dehydrogenation membrane reactors*, Seok-Jhin Kim, Yujun Liu, Jason S. Moore, Ravindra S. Dixit, John G. Pendergast, David S. Sholl, Christopher W. Jones, Sankar Nair, *Chemistry of Materials*, 28 (2016) 4387-4402
57. *Identification of high-CO₂-capacity cationic zeolites by accurate computational screening*, Hanjun Fang, Ambarish Kulkarni, Preeti Kamakoti, Rohan Awati, Peter I. Ravikovitch, and David S. Sholl, *Chemistry of Materials*, 28 (2016) 3887-3896
58. *Computational identification and experimental evaluation of metal-organic frameworks for xylene enrichment*, Jason A. Gee, Ke Zhang, Souryadeep Bhattacharyya, Jason Bentley, Meha Rungta, Jeevan S. Abichandani, David S. Sholl and Sankar Nair, *Journal of Physical Chemistry C*, 120 (2016) 12075-12082
59. *Effects of Open Metal Site Availability on Adsorption Capacity and Olefin/Paraffin Selectivity in the Metal-Organic Framework Cu₃(BTC)₂*, Jason Bentley, Guo Shiou Foo, Meha Rungta, Sangar Neeraj, Carsten Sievers, David S. Sholl, and Sankar Nair, *Industrial and Engineering Chemistry Research*, 55 (2016) 5043-5053
60. ***Seven Chemical Separations To Change The World*, David S. Sholl and Ryan P. Lively, *Nature*, 532 (2016), 435-437
61. *A Comprehensive Set of High-Quality Point Charges for Simulations of Metal-Organic Frameworks*, Dalar Nazarian, Jeffrey S. Camp, and David S. Sholl, *Chemistry of Materials*, 28 (2016) 785-793

62. *Transition State Theory methods to measure diffusion in flexible nanoporous materials: Application to a porous organic cage crystal*, Jeffrey Camp and David S. Sholl, *Journal of Physical Chemistry C*, 120 (2016) 1110-1120
63. *Effect of framework flexibility on C₈ aromatic adsorption at high loadings in metal-organic frameworks*, Jason A. Gee and David S. Sholl, *Journal of Physical Chemistry C*, 120 (2016) 370-376
64. *Computational characterization of defects in metal-organic frameworks: Spontaneous and water-induced point defects in ZIF-8*, Chenyang Zhang, Chu Han, David S. Sholl, and J. R. Schmidt, *Journal of Physical Chemistry Letters*, 7, (2016) 459-464
65. *Temperature and loading-dependent diffusion of light hydrocarbons in ZIF-8 as predicted through fully flexible molecular simulations*, Ross Verploegh, Sankar Nair and David S. Sholl, *Journal of the American Chemical Society*, 137 (2015) 15760-15771
66. *Propane dehydrogenation over In₂O₃-Ga₂O₃-Al₂O₃ Mixed Oxides*, Shuai Tan, Seok-Jhin Kim, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, John G. Prendergast, David S. Sholl, Sankar Nair, and Christopher W. Jones, *ChemCatChem*, 8 (2016) 214-221
67. *High T_c layered ferroelectric crystals by coherent spinodal decomposition*, Michael A. Susner, Alex Belianinov, Albina Borisevich, Qian He, Marius Chyasnavichyus, Hakan Demir, David S. Sholl, Panchapakesan Ganesh, Douglas L. Abernathy, Michael A. McGuire and Petro Maksymovch, *ACS Nano*, 9 (2015) 12365-12373
68. *Large-scale computational screening of binary intermetallics for membrane-based hydrogen separation*, Nita Chandrasekhar and David S. Sholl, *Journal of Physical Chemistry C*, 119 (2015) 26319-26326
69. *DFT-based force field development for noble gas adsorption in metal organic frameworks*, Hakan Demir, Jeffrey A. Greathouse, Chad L. Steiger, John J. Perry IV, Mark D. Allendorf and David S. Sholl, *Journal of Materials Chemistry A*, 3 (2015) 23539-23548
70. *Benchmarking density functional theory predictions of framework structures and properties in a chemically diverse test set of metal-organic frameworks*, Dalar Nazarian, P. Ganesh and David S. Sholl, *Journal of Materials Chemistry A*, 3 (2015) 22432-22440
71. **Defects in metal-organic frameworks: Challenge or opportunity?*, David S. Sholl and Ryan P. Lively, *Journal of Physical Chemistry Letters*, 6 (2015) 3437-3444
72. *Computational identification of descriptors for selectivity in syngas reactions on a Mo₂C catalyst*, Liwei Li and David S. Sholl, *ACS Catalysis*, 5 (2015) 5174-5185
73. *Predicting multicomponent adsorption: 50 years of the ideal adsorbed solution theory*, Krista S. Walton and David S. Sholl, *AIChE Journal*, 61 (2015) 2757-2762
74. *DFT-derived force fields for modeling hydrocarbon adsorption in MIL-47(V)*, Ambarish R. Kulkarni and David S. Sholl, *Langmuir*, 31 (2015) 8453-8468
75. *Efficient calculation of gas diffusivity in single-component and binary mixtures of spherical adsorbates in flexible 8MR zeolites*, Rohan V. Awati, Peter I. Ravikovitch, and David S. Sholl, *Journal of Physical Chemistry C*, 119 (2015) 16596-16605
76. *Prediction of adsorption properties of cyclic hydrocarbons in MOFs using DFT-derived force fields*, Jason A. Gee and David S. Sholl, *Journal of Physical Chemistry C*, 119 (2015) 16920-16926

77. *Modeling diffusion of linear hydrocarbons in silica zeolite LTA using transition path sampling*, Salah Eddine Boulfefel, Peter I. Ravikovitch, and David S. Sholl, *Journal of Physical Chemistry C*, 119 (2015) 15643-15653
78. *Catalytic propane dehydrogenation of In₂O₃-Ga₂O₃ mixed oxides*, Shuai Tan, Laura Briones Gil, Nachal Subramanian, David S. Sholl, Sankar Nair, Christopher W. Jones, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, John G. Prendergast, *Applied Catalysis A*, 498 (2015) 167-175
79. *Fluorinated carbide-derived carbon: More hydrophilic, yet apparently more hydrophobic*, Amir H. Farmahini, David S. Sholl, and Suresh K. Bhatia, *Journal of the American Chemical Society*, 137 (2015) 5969-5979
80. *Computational prediction of metal organic frameworks suitable for molecular infiltration as a route to development of conductive materials*, Xiaowa Nie, Ambarish Kulkarni, and David S. Sholl, *Journal of Physical Chemistry Letters*, 6 (2015) 1586-1591
81. *Molecular design of amorphous porous organic cages for enhanced gas storage*, J. D. Evans, D. M. Huang, M. R. Hill, C. J. Sumbly, D. S. Sholl, A. W. Thornton, and C. J. Doonan, *J. Phys. Chem. C* 119 (2015) 7746-7754
82. *Selection of surface coatings for high H₂ permeability group 5 metal membranes using first-principles calculations*, Rongshun Zhu, Shiqiang Hao, and David S. Sholl, *J. Phys. Chem. C* 119 (2015) 7848-7855
83. **Highly tunable molecular sieving and adsorption properties of mixed-linker zeolitic imidazolate frameworks*, Kiwon Eum, Krishna C. Jayachandrababu, Fereshteh Rashidi, Ke Zhang, Johannes Leisen, Samuel Graham, Ryan P. Lively, Ronald R. Chance, David S. Sholl, Christopher W. Jones and Sankar Nair, *Journal of the American Chemical Society*, 137 (2015) 4191-4197
84. *Impact of branching on the supramolecular assembly of thioethers on Au(111)*, Colin J. Murphy, Xuerong Shi, April D. Jewell, Allister F. McGuire, Darin O. Bellisario, Ashleigh E. Baber, Heather L. Tierney, Emily A. Lewis, David S. Sholl, and E. Charles H. Sykes, *Journal of Chemical Physics*, 142 (2015) 101915
85. *Material properties and operating configurations of membrane reactors for propane dehydrogenation*, Seung-Won Choi, Christopher W. Jones, Sankar Nair, David S. Sholl, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, and John G. Prendergast, *AIChE Journal*, 61 (2015) 922-935
86. ***The materials genome in action: identifying the performance limits for methane storage*, Cory M. Simon, Jihan Kim, Diego A. Gomez-Gualdron, Jeffrey S. Camp, Yongchul G. Chung, Richard L. Martin, Rocio Mercado, Michael W. Deem, Dan Gunter, Maciej Haranczyk, David S. Sholl, Randall Q. Snurr, and Berend Smit, *Energy & Environmental Science* 8 (2015) 1190-1199
87. *First-principles screening of complex transition metal hydrides for high temperature applications*, Kelly M. Nicholson and David S. Sholl, *Inorganic Chemistry*, 53 (2014) 11833-11848
88. *First-principles prediction of new complex transition metal hydrides for high temperature applications*, Kelly M. Nicholson and David S. Sholl, *Inorganic Chemistry*, 53 (2014) 11849-11860
89. **Computation-ready, Experimental Metal-Organic Frameworks: A tool to enable high-throughput screening of nanoporous crystals*, Yongchul G. Chung, Jeffrey

- Camp, Maciej Haranczyk, Benjamin J. Sikora, Wojciech Bury, Vaiva Krungleviciute, Taner Yildirim, Omar K. Farha, David S. Sholl, and Randall Q. Snurr, *Chemistry of Materials*, 26 (2014) 6185-6192
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336. ***Diffusion of Clusters of Atoms and Vacancies on Surfaces and the Dynamics of Diffusion Driven Cluster Coarsening*, David S. Sholl and Rex T. Skodje, *Physical Review Letters* **75** (1995) 3158.
337. *Exact Solutions of the Monomer-Monomer Reaction: Segregation, Poisoning, and Interface Evolution*, David S. Sholl and Rex T. Skodje, *Physical Review E* **53** (1995) 335.
338. *Surface Diffusion of H and CO on Cu/Ru(001): Evidence for Long-Range Trapping by Copper Islands*, David E. Brown, David S. Sholl, Rex T. Skodje, and Steven M. George, *Chemical Physics* **201** (1995) 273.
339. *Kinetic Phase Transitions and Bistability in a Model Surface Reaction I: Monte Carlo Simulations*, David S. Sholl and Rex T. Skodje, *Surface Science* **334** (1995) 295.
340. *Kinetic Phase Transitions and Bistability in a Model Surface Reaction II: Spatially Inhomogeneous Theories*, David S. Sholl and Rex T. Skodje, *Surface Science* **334** (1995) 305.
341. *Comment on 'A Theoretical Stochastic Model for the $A+1/2B_2 \rightarrow 0$ Reaction'* [*J. Chem. Phys.* 98 (1993) 10017], David S. Sholl and Rex T. Skodje, *Journal of Chemical Physics* **101** (1994) 855.
342. *Diffusion of Xenon on a Platinum Surface: The Influence of Correlated Flights*, David S. Sholl and Rex T. Skodje, *Physica D* **71** (1994) 168.
343. *Optimal Resolution in Maximum Entropy Image Reconstruction from Projections with Multigrid Acceleration*, Mark A. Limber, Tom A. Manteuffel, Stephen F. McCormick, and David S. Sholl, *Proc. Of the Sixth Copper Mountain Conference on Multigrid Methods* (1993) 361.
344. *A Semi-Lagrangian Approach to the Shallow Water Equations*, J. R. Bates, Stephen F. McCormick, John Ruge, David S. Sholl, and Irad Yavneh *Proc. Of the Sixth Copper Mountain Conference on Multigrid Methods* (1993) 593.
345. *Perturbative Calculation of Superperiod Recurrence Times in Nonlinear Chains*, David S. Sholl and B. I. Henry, *Physics Letters A* **159** (1991) 21.
346. *Recurrence Times in Cubic and Quartic Fermi-Pasta-Ulam Chains: A Shifted-Frequency Analysis*, David S. Sholl and B. I. Henry, *Physical Review A* **44** (1991) 6364.
347. *Modal Coupling in One-Dimensional Anharmonic Chains*, David S. Sholl, *Physics Letters A* **149** (1990) 253.

Books

Non-fiction

Density Functional Theory: A Practical Introduction, David S. Sholl and Jan Steckel, John Wiley & Sons, 2009 (ISBN: 978-0470373170).

- Turkish edition published in 2014.
- Japanese and Chinese editions published in 2015.
- > 1000 citations reported by Google Scholar.

Fiction

Polyphony, David Sholl, Sleeping Kangaroo Publishers, 2018 (ASIN: B07D1TR6NJ)

Patents

1. MOF nanocrystals, A. Brown, S. Nair, C. Carson, S. Nair, D. S. Sholl, US Patent 8,668,764, Issued March 11, 2014
2. Screening metal organic framework materials, E. Haldoupis, S. Keskin, S. Nair., D. S. Sholl, US Patent 8,725,482, Issued May 13, 2014

Departmental Seminars and Invited Presentations

1. Gordon Research Conference on Nanoporous Materials, Andover, NH, August 2019
2. Department of Chemical Engineering, New Mexico State University, Las Cruces, NM, April 2019
3. Department of Chemical Engineering, University of Arkansas, April 2019
4. Inaugural Ma Lecture, Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA, April 2019
5. Symposium on New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations and Theory, ACS National Meeting, Orlando, FL, April 2019
6. George Olah Award Symposium in Honor of Chunshan Song, ACS National Meeting, Orlando, FL, April 2019
7. Department of Chemical Engineering, University of New Hampshire, April 2019
8. Division of Physical Sciences, Pacific Northwest National Laboratory, March 2019
9. Department of Chemical Engineering, Oklahoma State University, December 2018
10. University College London, London, UK, December 2018
11. Department of Chemical Engineering, Virginia Commonwealth University, October 2018
12. Department of Chemical Engineering, Drexel University, November 2018
13. Department of Chemical Engineering and Materials Science, University of Alberta, Edmonton, Alberta, October 2018
14. Parr Lecture, Department of Chemical and Biomolecular Engineering, University of Illinois, Champaign, IL, September 2018
15. Plenary Lecture, 15th International Conference on Inorganic Membranes, Dresden, Germany, June 2018
16. Department of Nanoengineering, UCSD, La Jolla, CA, April 2018
17. Department of Chemical Engineering, UC Berkeley, Berkeley, CA, March 2018
18. Department of Chemical Engineering, South Dakota School of Mines, March 2018

19. Plenary Lecture, 2018 US DOE Basic Energy Sciences Separation Science PI Meeting, Gaithersburg, MD, February 2018
20. Material Informatics Seminar, National Institute of Standards, Gaithersburg, MD, February 2018
21. New Vistas in Molecular Thermodynamics, Humboldt Kolleg, Berkeley, CA, January 2018
22. NAS Committee on Reproducibility and Replicability in Science, Washington DC, December 2017
23. Sustainable Engineering Forum Plenary Session, AIChE Annual Meeting, Minneapolis, MN, November 2017
24. Department of Chemical Engineering, MIT, Boston, MA, October 2017
25. Department of Chemical Engineering, Tulane University, New Orleans, LA, September 2017
26. Department of Chemical Engineering, Kansas State University, Manhattan, KS, September 2017
27. Department of Chemical & Petroleum Engineering, University of Kansas, Lawrence, KS, September 2017
28. Sandia National Laboratory, Albuquerque, NM, August 2017
29. ORNL Materials Informatics Workshop, Oak Ridge National Lab, Oak Ridge, TN, August 2017
30. ASEE Summer School for Chemical Engineering Faculty, Raleigh, NC, August 2017
31. Keynote Lecture, Australian CCS Research Conference, Melbourne, VIC, Australia, June 2017
32. AINST Distinguished Seminar, University of Sydney, Sydney, NSW, Australia, June 2017
33. Department of Chemical Engineering, University of New South Wales, Kensington, NSW, Australia, June 2017
34. Department of Physics Colloquium, University of Queensland, Brisbane, QLD, Australia, June 2017
35. CSIRO and University of Monash Department of Chemistry, Clayton, VIC, Australia, May 2017
36. Mieyungah Public Lecture, University of Melbourne, Melbourne, Australia, May 2017
37. Tau Beta Pi Initiates Dinner talk, Georgia Institute of Technology, Atlanta, GA, April 2017
38. Department of Chemical Engineering, University of California Davis, Davis, CA, March 2017
39. Department of Chemical Engineering, Colorado School of Mines, Golden, CO, January 2017
40. Robin H. Stokes Lecture, University of New England, Armidale, NSW, Australia, December 2016
41. Plenary Lecture, Fundamentals and Applications of Advanced Porous Materials Conference, Adelaide, South Australia, Australia, December 2016
42. Department of Chemical and Biological Engineering, University of Delaware, Newark, DE, December 2016

43. Department of Chemical Engineering and Materials Science, Cal Poly Pomona, Pomona, CA, November 2016
44. Department of Chemical Engineering, Texas Tech, Lubbock, TX, November 2016.
45. Georgia Research Alliance Eminent Scholars Annual Meeting, Atlanta, GA, October 2016.
46. Symposium on Supramolecular Assemblies and Metal-Organic Frameworks, SERMACS, Columbia, SC, October 2016.
47. University of Houston Honors College, Houston, TX, October 2016
48. School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, September 2016
49. Department of Chemical Engineering, University College Dublin, Dublin, Ireland, September 2016
50. International Zeolite Membrane Meeting 2016, Dalian, China, August 2016
51. University of Seoul, Seoul, Korea, August 2016
52. Seoul National University, Seoul, Korea, August 2016
53. Board for Chemical Sciences and Technology, National Academy of Sciences, Irvine, CA, August 2016.
54. Gordon Conference on Membranes, New London, NH, August 2016.
55. Gulf Coast and Latin America Scientists Association Seminar Series, Dow Chemical, Freeport, TX, May 2016
56. Savannah River National Laboratory, Aiken, SC, May 2016
57. Symposium on Design, Synthesis and Applications of Advanced Porous Materials, Pacifichem, Honolulu, HI, December 2015
58. Symposium on Data Mining and Machine Learning Meets Experiment and First-principles Simulation for Materials Discovery, Pacifichem, Honolulu, HI, December 2015
59. Symposium on Safety in the Academic Research Laboratory, Pacifichem, Honolulu, HI, December 2015
60. Department of Chemical, Petroleum and Materials Engineering, University of Southern California, Los Angeles, CA, October 2015
61. Department of Chemical and Biomolecular Engineering, University of California Riverside, Riverside, CA, October 2015
62. Department of Chemical and Biomolecular Engineering, University of California Irvine, Irvine, CA, October 2015
63. Department of Chemical Engineering, University of Houston, Houston, TX, October 2015
64. Department of Chemical and Biomolecular Engineering, University of Florida, Gainesville, FL, September 2015
65. Department of Chemical and Biological Engineering, University of Buffalo, Buffalo, NY, September 2015
66. Department of Chemical Engineering, Northeastern University, Boston, MA, August 2015
67. Multiscale Porosity From Laboratory To Industrial Application, 2nd Micromeritics Workshop, Massachusetts Institute of Technology, Cambridge, MA, August 2015
68. School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, August 2015

69. US-Korea Conference on Science, Technology, and Entrepreneurship , Atlanta, GA, July 2015
70. DOE BES Catalysis Contractors Workshop, Annapolis, MD, July 2015
71. Gordon Research Conference on Hydrogen Metal Systems, Stonehill College, MA, July 2015
72. Workshop on Metal-Organic Frameworks, Telluride Scientific Research Conference, Telluride, CO, June 2015.
73. CECAM Workshop on Defects and Disorder in Metal-Organic Frameworks, Chimie ParisTech, Paris, France, June 2015
74. 3M Tech Talk, Minneapolis, MN, May 2015
75. UOP Technical Seminar, Des Plaines, IL, May 2015
76. Department of Chemical Engineering, University of Illinois at Chicago, Chicago, IL, May 2015
77. Symposium on Genomic Approaches to Materials, 249th ACS National Meeting, Denver, CO, March 2015
78. Symposium on Environmental Applications of Metal-Organic Frameworks, 249th ACS National Meeting, Denver, CO, March 2015
79. Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, March 2015
80. Department of Chemical and Biomolecular Engineering, University of South Florida, Tampa, FL, February 2015
81. Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD, December 2014
82. Chinese American Chemical Society Banquet, Atlanta, GA, November 2014
83. Molecular Thermodynamics Plenary Session, AIChE Annual Meeting, Atlanta, GA, November 2014
84. Fossil Fuels Plenary Session, AIChE Annual Meeting, Atlanta, GA, November 2014
85. Department of Chemical and Biomolecular Engineering, Columbia University, New York, NY, November 2014
86. Adsorption Technologies Group, Sasol, Sasolburg, South Africa, November 2014
87. Particle Technology Workshop, University of Cape Town, Cape Town, South Africa, November 2014
88. ExxonMobil Applied Materials Symposium, Hershey, PA, October 2014
89. Department of Chemical and Biomolecular Engineering, University of Colorado, Boulder, CO, October 2014
90. Trotter Distinguished Lecture, Department of Chemical Engineering, University of Tennessee, October 2014
91. Symposium on MOFs for Applications, 248th ACS National Meeting, San Francisco, CA, August 2014
92. School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, August 2014
93. Metal Hydrogen 2014, Manchester, UK, July 2014
94. Department of Chemical Engineering, Imperial College London, London, UK, July 2014
95. Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, July 2014

96. Department of Chemistry, National University of Singapore, Singapore, July 2014
97. Department of Chemical Engineering, University of Melbourne, Melbourne, Australia, June 2014
98. International Conference on Inorganic Membranes (keynote address), Brisbane, Australia, June 2014
99. MRS Spring Meeting, San Francisco, CA, April 2014
100. Florida AVS Meeting, Orlando, FL, March 2014
101. J. H. Hopps 5th Annual Training Symposium, Morehouse College, Atlanta, GA, February 2014
102. Dow Chemical Company, Freeport, TX, January 2014
103. School of Chemistry Colloquium, Georgia Institute of Technology, Atlanta, GA, October 2013
104. Physical Chemistry Seminar, University of Wisconsin, Madison, WI, October 2013
105. Department of Chemical and Biomolecular Engineering, Northwestern University, Evanston, IL, October 2013
106. International Zeolite Membrane Meeting, Jeju Island, South Korea, June 2013
107. Workshop on Adsorption in Compliant Solids, Paris, France, June 2013
108. International Conference on Energy and Sustainability, Hang Zhou, China, May 2013
109. Department of Physics, Oberlin College, Oberlin, OH, May 2013
110. Symposium on CO₂ Capture and Utilization, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013
111. Symposium on Hydrogen Production, Storage, and Utilization, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013
112. Symposium on Identification of Environmental Abiotic and Biotic Reactions Using Computational Chemistry, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013
113. Department of Chemistry, University of Florida, February 2013
114. Georgia Tech Clean Energy Speaker Series, Atlanta, GA, February 2013
115. CSIRO, Clayton, Victoria, Australia, December 2012
116. Dept. of Chemical Engineering, University of Queensland, December 2012
117. Pacific Northwest National Laboratory, December 2012
118. Department of Chemical Engineering, Clemson University, November 2012
119. Physical Chemistry seminar, Department of Chemistry, University College London, London, UK, October 2012
120. Air Capture: Developing Technologies for Carbon Recycling and Negative Emissions, Institution of Mechanical Engineering, London, UK, October 2012
121. MOF2012 Keynote Lecture, Edinburgh, UK, September 2012
122. Foundations of Molecular Modeling and Simulations, Portland, OR, July 2012.
123. NETL ORD Seminar, National Energy Technology Laboratory, Pittsburgh, PA, June 2012.
124. Symposium on Gas Capture Materials, Canadian Society of Chemistry Conference, Calgary, AB, May 2012
125. CNMS Theory Seminar, Oak Ridge National Laboratory, Oak Ridge, TN, May 2012

126. ORNL Reactor Off Gas Group, Oak Ridge National Laboratory, Oak Ridge, TN, May 2012
127. Washington University in St. Louis, Department of Energy, Environment, and Chemical Engineering, April 2012
128. University of South Carolina, Department of Chemical Engineering, Columbia, SC, March 2012
129. Materials Modeling Group, Intel Corporation, Santa Clara, CA, March 2012
130. Symposium on Non-adiabatic Dynamics: Surface Hopping and Beyond (invited talk), 243rd ACS National Meeting, San Diego, CA, March 2012
131. Symposium on High-Throughput Screening Approaches for Catalysts Discovery and Optimization (invited talk), 243rd ACS National Meeting, San Diego, CA, March 2012
132. University of California Berkeley, Carbon Capture Program, February 2012
133. Stanford University, Department of Energy Resources Engineering, February 2012
134. MADE@GT Symposium on Materials Design, Atlanta, GA, November, 2011
135. Georgia Research Alliance Eminent Scholars Annual Meeting, Atlanta, GA, October 2011
136. Department of Chemical Engineering Seminar, University of Kentucky, Louisville, KY, October 2011.
137. Sandia National Laboratory, Microfluidics Department, Livermore, CA, September 2011.
138. Nanoporous Materials VI (plenary presentation), Banff, Canada, August 21-24, 2011.
139. National Summit on Advancing Clean Energy Technologies (invited panelist), Washington DC, May 2011.
140. Workshop on Materials Design in Chemical Compound Space, Institute for Pure and Applied Mathematics, UCLA, Los Angeles, CA, May 2011
141. Symposium on Applications of Metal-Organic Frameworks, MRS Spring Meeting, San Francisco, CA, April 2011
142. APS March Meeting, Dallas, TX, March 2011
143. Department of Chemical Engineering, National University of Singapore, Singapore, February 2011
144. Institute for Atom-efficient Chemical Transformations Workshop, Northwestern University, Evanston, IL, November 2010
145. COMSEF Plenary Session, AIChE Annual Meeting, Salt Lake City, November 2010
146. Open Forum of the Energy and Environment, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, October 2010
147. Neutrons in Catalysis Workshop, Oak Ridge National Laboratory, September 2010
148. Symposium on Nanoporous Materials for Environmental Applications, ACS National Meeting, Boston, August 2010
149. 5th International Zeolite Membrane Meeting, Loutraki, Greece, May 2010.

150. Department of Chemical and Bioengineering, University of Washington, Seattle, WA, May 2010.
151. Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, April 2010.
152. Department of Chemical Engineering, The Pennsylvania State University, State College, PA, April 2010.
153. Keynote Lecture, Symposium on Advances in Membrane Science and Technology, ACS National Meeting, San Francisco, March 2010.
154. Dept. of Chemical Engineering, Texas A&M University, College Station, TX, January 2010.
155. Oak Ridge National Laboratory, Computational Materials Division, Knoxville, TN, January 2010.
156. Thin Films Division, AVS 56th International Symposium, San Jose, November 2009.
157. Dept. of Chemical Engineering, Clemson University, October 2009.
158. DOE Computational Materials Science Network Workshop, Denver, CO, October, 2009.
159. XVIII International Materials Research Congress, Cancun, Mexico, August 2009.
160. US-China Workshop on Surface Science and Heterogeneous Catalysis, Dalian, China, June 2009.
161. Savannah River National Laboratory, Materials Division, Aiken, SC, June 2009.
162. Swedish-American Entrepreneurial Days, Keynote Address, Savannah, GA, April 2009.
163. Emerson Center Annual Symposium, Emory University, March 2009.
164. Dept. of Chemical Engineering, University of Louisville, Louisville, KY, February 2009
165. Center for Simulational Physics, 22nd Annual Workshop, University of Georgia, Athens, GA, February 2009
166. Dept. of Chemical Engineering, University of New South Wales, Sydney, NSW, Australia, December 2008.
167. Dept. of Physics, University of Sydney, Sydney, NSW, Australia, December 2008.
168. Dept of Chemical Engineering, University of Melbourne, Melbourne, Victoria, Australia, December 2008
169. CSIRO Energy Research Center, Brisbane, Queensland, Australia, December 2008
170. Future Directions in Transport, Centennial Symposium, AIChE Annual Meeting, Philadelphia, November 2008.
171. Department of Chemical Engineering, University of Maine, Bangor, ME, October 2008
172. University of Queensland Physics Summer School, Stradbroke Island, Queensland, Australia, December 2008.
173. Center for Nanoscale Materials, Argonne National Laboratory, Chicago, IL, October 2008
174. Center for Simulational Physics, University of Georgia, Athens, GA, October 2008

175. College of Engineering, Peking University, Beijing, China, May 2008.
176. Department of Chemistry, Tsinghua University, Beijing, China, May 2008.
177. Department of Chemical Engineering, Beijing University of Chemical Technology, Beijing, China, May 2008.
178. Department of Chemistry, Emory University, Atlanta, GA, April 2008.
179. Thermodynamics in Chemical Engineering: Prospects and Perspectives, AIChE Spring Meeting, New Orleans, LA, April 2008.
180. Computational Methods and Molecular Modeling in Fuel Chemistry, ACS National Meeting, New Orleans, LA, April 2008.
181. Arthur W. Adamson Award for Distinguished Service of Surface Chemistry: Symposium in Honor of Francisco Zaera, ACS National Meeting, New Orleans, LA, April 2008.
182. Department of Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ, November 2007.
183. Department of Materials Science and Engineering, University of Illinois, Champaign, IL, November 2007.
184. MESD Plenary Session, AIChE Annual Meeting, Salt Lake City, UT, November 2007.
185. CECAM Workshop on Chirality at Surfaces, Lyons, France, October 2007.
186. Symposium on Advanced Materials for Conversion and Separations in Energy Applications, ACS National Meeting, Boston, MA, August 2007.
187. Symposium on Hydrogen Storage and Fuel Cell Technology, ACS National Meeting, Boston, MA, August 2007.
188. Gordon Conference on Hydrogen in Metals, Waterville, Maine, July 10, 2007.
189. Department of Chemical Engineering, Oklahoma University, April 19, 2007
190. Symposium on Capturing Complexity in Physical Sciences Simulation, ACS National Meeting, Chicago, IL, March 27, 2007
191. Symposium on Implications and Applications of Chirality in Physical Chemistry, ACS National Meeting, Chicago, IL, March 28, 2007
192. Department of Chemical Engineering and Materials Science, University of Minnesota, January 23, 2007.
193. Department of Chemistry, Carleton College, January 12, 2007.
194. Biosecurity and Nanosciences Laboratory, Lawrence Livermore National Laboratory, January 10, 2007.
195. COMSEF Plenary Session, AIChE Annual Meeting, San Francisco, California, November 12-16, 2006
196. Department of Chemical Engineering, Carnegie Mellon University, November 2, 2006
197. Department of Chemical Engineering, Vanderbilt University, October 30, 2006.
198. Department of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia, October 18, 2006
199. Metal-Hydrogen 2006, Maui, Hawaii, October 1-6, 2006
200. Symposium on Challenges for the Hydrogen Economy: Storage Science and Technology, ACS National Meeting, San Francisco, California, September 10-14, 2006.

201. Symposium on Chirality and Enantioselectivity at Surfaces, ACS National Meeting, San Francisco, California, September 10-14, 2006.
202. Symposium on Computational Materials Design in Chemical Industries, ACS National Meeting, San Francisco, California, September 10-14, 2006.
203. Gordon Research Conference on Membranes: Materials and Processes, New London, NH, August 6-11, 2006.
204. Gordon Research Conference on Physical Metallurgy, Plymouth, NH, July 23-26, 2006.
205. Gordon Research Conference on Chemistry at Interfaces, Biddeford, Maine, July 9-14, 2006.
206. Department of Physics, University of Sydney, Sydney, NSW, Australia, May 19, 2006.
207. 135th TMS Annual Meeting, March 12-16, 2006, San Antonio, TX.
208. Center for Low Emission Technologies, University of Queensland, Brisbane Australia, December 2005.
209. ARC Center for Functional Nanomaterials 2nd Annual Meeting, Noosa Heads, Australia, December 2005.
210. Department of Chemical Engineering, University of Melbourne, Melbourne, Australia, November 2005.
211. Center for Molecular Modeling, Swinburne University, Melbourne, Australia, November 2005.
212. China/Japan/USA Joint Chemical Engineering Meeting, Beijing, China, October 11-13, 2005.
213. Department of Chemical Engineering, University of Newcastle, Newcastle, Australia, October 2005.
214. CSIRO Energy Center, Newcastle, Australia, October 2005.
215. ExxonMobil Corporate Research, Annandale, NJ, October 2005.
216. Nanoscale Science and Technology Center, Griffith University, Brisbane, Australia, August 2005.
217. Department of Chemical Engineering and Materials Science, Arizona State University, Tempe, AZ, April 2005.
218. Department of Chemical Engineering, City College of New York, New York, NY, February 2005.
219. Department of Materials Science, University of Pittsburgh, Pittsburgh, PA, February 2005.
220. Department of Chemical Engineering, University of Colorado, Boulder, CO, January 2005.
221. Workshop on Molecular and Particle Processes at Solid Surfaces, San Luis, Argentina, November 2004.
222. ExxonMobil Corporate Research, Annandale, NJ, September 2004.
223. 3rd International Zeolite Membrane Meeting, Breckenridge, CO, July 2004.
224. van't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, Holland, May 2004.
225. Surface Science Center, University of Liverpool, Liverpool, UK, May 2004.
226. Department of Chemistry, University of Cardiff, Cardiff, UK, May 2004.

227. Department of Chemistry, University of Sydney, Sydney, NSW, Australia, May 2004.
228. Department of Physics, University of New England, Armidale, NSW, Australia, May 2004.
229. Department of Chemical Engineering, University of Queensland, Brisbane, Qld., Australia, April 2004.
230. Department of Chemical Engineering, Purdue University, West Lafayette, IN, March 2004.
231. Third San Luis Symposium on Surface Science, Merida, Venezuela, March 2004.
232. Department of Chemistry, Wake Forest University, Winston-Salem, NC, February 2004.
233. Department of Chemistry, Duquesne University, Pittsburgh, PA, January 2004.
234. Surface Analysis session, FACSS 2003 Annual Meeting, Ft. Lauderdale, FL, October 2003.
235. Department of Materials Science and Engineering, University of Florida, Gainesville, FL, October 2003.
236. Department of Chemical Engineering, University of Florida, Gainesville, FL, October 2003.
237. Department of Chemical Engineering, University of Buffalo, Buffalo, NY, October 2003.
238. CECAM Workshop on Simulation of Zeolites: Towards In Silico Design, Lyons, France, October 2003.
239. Department of Physics, Indiana University of Pennsylvania, Indiana, PA, September 2003.
240. Chiral Surfaces Symposium, ACS National Meeting, New Orleans, LA, March 2003.
241. Mechanistic Surface Chemistry Symposium, ACS National Meeting, New Orleans, LA, March 2003
242. Department of Chemical Engineering, University of Missouri at Rolla, January 2003.
243. Pittsburgh-Cleveland Catalysis Society, Pittsburgh, PA, December 2002.
244. Department of Chemical Engineering, University of Wisconsin, December 2002.
245. CAST Plenary Session, AIChE Annual Meeting, Indianapolis, IN, November 2002.
246. Department of Chemical Engineering, University of Delaware, October 2002.
247. Pittsburgh AIChE Chapter, October 2002.
248. Materials Research Seminar, Department of Chemical Engineering, The Pennsylvania State University, October 2002.
249. Chemical Physics/Physical Chemistry Seminar, Departments of Chemistry and Physics, University of Maryland, September 2002
250. GE Corporate Research and Development, Albany, NY, September 2002
251. TDA Inc., Wheatridge, CO, June 2002.
252. National Renewable Energy Laboratory, June 2002.
253. Computational Materials and Biology Group, Sandia National Laboratory, Albuquerque, NM, June 2002.

254. Atomic and Molecular Physics Group, T-Division, Los Alamos National Laboratory, May 2002.
255. Department of Chemical Engineering, University of Massachusetts – Amherst, April 2002.
256. Department of Chemical Engineering, University of Akron, February 2002.
257. Air Products R&D Division, January 2002.
258. Department of Chemical Engineering, University of California at Santa Barbara, Santa Barbara, CA, November 2001.
259. Department of Chemistry, Kent State University, Kent, OH, September 2001.
260. Midwest Thermodynamics and Statistical Mechanics Meeting, East Lansing, MI, May 2001.
261. Computational Materials and Biology Group, Sandia National Laboratory, Albuquerque, NM, December 2000.
262. Department of Chemical Engineering, University of Colorado, October 2000.
263. Department of Applied Mathematics, University of Colorado, October 2000.
264. ExxonMobil Corporate Research Division, Annandale, NJ, June 2000.
265. Air Products and Chemicals Technology Division, Allentown, PA, June 2000.
266. Department of Chemical Engineering, University of Tennessee, April 2000.
267. ACS National Meeting, San Francisco, CA, March 2000 (invited presentation).
268. Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA, October 1999.
269. Condensed Matter Seminar, Department of Physics, Carnegie Mellon University, Pittsburgh, PA, October 1998
270. Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, PA, September 1998
271. Department of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, March 1997.
272. Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA, February 1997.
273. Department of Chemistry, Iowa State University, Ames, IA, January 1997.
274. Department of Applied Mathematics, University of Colorado, Boulder, CO, November 1995.
275. Physics Department, University of New England, Armidale, NSW, Australia, December 1993.
276. Department of Physics and Theoretical Physics, Australian National University, Canberra, ACT, Australia, March 1991.

Other Presentations (partial list)

1. AIChE Annual Meeting, Pittsburgh, PA, October 2018 (12 contributed presentations and 2 posters)
2. AIChE Annual Meeting, Minneapolis, MN, October 2017 (12 contributed presentations)
3. AIChE Annual Meeting, San Francisco, CA, November 2016 (5 contributed presentations)
4. AIChE Annual Meeting, Salt Lake City, UT, November 2015 (2 contributed presentations)

5. AIChE Annual Meeting, Atlanta, GA, November 2015 (14 contributed presentations)
6. International Conference on Inorganic Membranes, Brisbane, Australia, June 2014 (1 contributed presentation)
7. Nano-7, Niagara Falls, Ontario, June 2014 (1 contributed presentation)
8. AIChE Annual Meeting, San Francisco, CA, November 2013 (8 contributed presentations)
9. AIChE Annual Meeting, Pittsburgh, PA, October 2012 (9 contributed presentations)
10. 243rd ACS National Meeting, San Diego, CA, March 2012 (1 contributed presentations, 1 invited presentation given by G. Parkinson)
11. 17th Symposium on Separation Science and Technology for Energy Applications, Nashville, TN, October 2011 (2 contributed presentation)
12. AIChE Annual Meeting, Minneapolis, MN, October 2011 (7 contributed presentations)
13. ACS National Meeting, Denver, CO, August 2011 (1 invited presentation given by K. Walton)
14. Gordon Conference on Nanoporous Materials (2 posters)
15. North American Membrane Society Meeting, Las Vegas, NV, June 2011 (2 contributed presentations)
16. MRS Spring Meeting, San Francisco, CA, April 2011 (1 contributed presentation)
17. ACS National Meeting, Anaheim, CA, March 2011 (3 contributed presentations)
18. AIChE Annual Meeting, Salt Lake City, UT, November 2010 (4 contributed presentations)
19. NETL CO₂ Technology Meeting, Pittsburgh, PA, September 2010 (1 poster)
20. MOF2010, Marseille, France, September 2010 (1 contributed presentation, 1 poster)
21. ACS National Meeting, Boston, MA, August 2010 (3 contributed presentations)
22. ACS National Meeting, San Francisco, CA, March 2010 (2 contributed presentations)
23. 13th IACS International Conference on Surface and Colloid Science, New York, NY, June 2009 (1 contributed presentation)
24. NAMS 2009, Charleston, SC, June 2009 (2 contributed presentations)
25. ACS National Meeting, Salt Lake City, UT, March 2009 (2 contributed presentations)
26. APS March Meeting, Pittsburgh, PA, March 2009 (3 contributed presentations)
27. MRS Fall Meeting, Boston, MA, December 2008 (1 contributed presentation)
28. AIChE Annual Meeting, Philadelphia, PA, November 2008 (8 contributed presentations)
29. ASME Energy Nanotechnology Meeting, Jacksonville, FL, August 2008 (1 contributed presentation)
30. Metal Hydrogen 2008, Reykjavik, Iceland, June 2008 (2 contributed presentations, 1 poster)
31. ACS National Meeting, New Orleans, LA, April 2008 (1 contributed presentation)
32. National Hydrogen Association Annual Meeting, Sacramento, CA, March 2008 (1 contributed presentation, 1 poster)
33. ACS National Meeting, Boston, MA, August 2007 (7 contributed presentations)
34. North American Membrane Society Annual Meeting, Orlando, FL, May 14-16, 2007 (2 contributed presentations)
35. PCCS Spring Meeting, Morgantown, WV (3 contributed presentations)

36. 2nd International Workshop on In-situ Study and Development of Processes Involving Porous Materials, Thessalonika, Greece, February 24-28, 2007 (poster)
37. AIChE Annual Meeting, November 2006, San Francisco, CA (3 contributed presentations)
38. Metal-Hydrogen 2006, Maui, Hawaii, October 1-6, 2006 (contributed presentation)
39. 2006 Midwest Thermodynamics and Statistical Mechanics Meeting, Akron, OH, May 25-26, 2006 (3 presentations)
40. PCCS Fall Meeting, Pittsburgh, PA, December 9, 2005
41. China/Japan/USA Joint Chemical Engineering Meeting, Beijing, China, October 11-13, 2005 (contributed presentation)
42. W. E. Heraeus Seminar on Hydrogen Storage with Novel Nanomaterials, Bad Honnef, Germany, 23-27 October, 2005
43. ACS National Meeting, Washington, DC, August 28-September 1, 2005 (1 presentation, 2 posters)
44. Gordon Conference on Zeolitic and Layered Materials, South Hadley, MA, July 3-8, 2005 (poster).
45. 2005 Midwest Thermodynamics and Statistical Mechanics Meeting (3 presentations)
46. 19th North American Catalysis Society Meeting, Philadelphia, PA, May 22-27, 2005
47. PCCS Spring Meeting, Pittsburgh, PA, June 2005 (3 presentations)
48. ACS National Meeting, San Diego, CA, March 2005.
49. AIChE Annual Meeting, Austin, TX, November 2004 (7 presentations)
50. 2004 ASM Materials Solutions Conference, Columbus, OH, October 18-20, 2004.
51. 8th International Conference on Inorganic Membranes, Cincinnati, OH, June 2004 (4 presentations)
52. PCCS Spring Meeting, Pittsburgh, PA, June 2004 (2 presentations).
53. 2004 Midwest Thermodynamics and Statistical Mechanics Meeting (3 presentations).
54. ACS National Meeting, Anaheim, CA, March 2004 (4 presentations).
55. APS March Meeting, Montreal, Canada, March 2004.
56. AVS 50th International Symposium, Baltimore, MD, November 2003.
57. AIChE 2003 Annual Meeting, San Francisco, CA, November 16-21, 2003 (5 presentations)
58. 63rd Physical Electronics conference, Ithaca, NY, June 16-18, 2003.
59. 2003 Midwest Thermodynamics and Statistical Mechanics Meeting, Columbus, OH May 28-29, 2003 (3 presentations)
60. 2003 North American Membrane Society Meeting, Jackson Hole, WY, May 19-21, 2003 (2 presentations)
61. NASA Astrobiology General Institute Meeting, Tempe, AZ, Feb 10-12, 2003.
62. AIChE National Meeting, Indianapolis, IN, November 3-8, 2002 (7 presentations)
63. AVS 49th International Symposium, Denver, CO, November 3-8, 2002 (2 presentations)
64. ACS National Meeting, Boston, MA, August 17-21, 2002
65. American Conference on Theoretical Chemistry, Champion, PA, July 13-18, 2002 (2 posters)
66. 62nd Physical Electronics conference, Atlanta, GA, June 12-14, 2002.
67. 2002 Midwest Thermodynamics and Statistical Mechanics Meeting, Pittsburgh, PA, May 13-14, 2002 (4 presentations)

68. 2002 Pittsburgh-Cleveland Catalysis Society Symposium, Pittsburgh, PA, May 9-10, 2002 (2 presentations)
69. ACS National Meeting, Orlando, FL, April 7-11, 2002 (3 presentations)
70. APS March Meeting, Indianapolis, IN, March 18-22, 2002 (3 presentations)
71. AIChE National Meeting, Reno, NV, November 4-9, 2001 (4 presentations)
72. International Workshop on Zeolitic and Microporous Membranes, Purend, The Netherlands, July 2001 (poster).
73. 7th International Conference on Fundamentals of Adsorption, Nagasaki, Japan, May 20-25, 2001.
74. North American Membrane Society Annual Meeting, Lexington, KY, May 2001.
75. ACS Surfaces and Colloids Symposium, Pittsburgh, PA, June 2001 (2 presentations)
76. 2001 Midwest Thermodynamics and Statistical Mechanics Meeting, East Lansing, MI, May 2001.
77. MRS Spring Meeting, San Francisco, CA, April 2001 (3 presentations)
78. ACS National Meeting, San Diego, CA, March 2001 (3 presentations)
79. AIChE National Meeting, Los Angeles, CA, November 2000 (3 presentations).
80. ACS Colloids and Surfaces Symposium, Lehigh, PA, June 2000 (3 presentations)
81. Access in Nanoporous Materials II, Banff, Alberta, May 2000 (1 presentation & 1 poster)
82. 2000 Midwest Thermodynamics and Statistical Mechanics Meeting, Minneapolis, MN, May 2000.
83. ACS national meeting (3 presentations), San Francisco, CA, March 2000.
84. Workshop on Nanotribology: Critical Assessment and Research Needs, Gaithersburg, MD, March 2000 (poster).
85. AIChE National Meeting (6 presentations), Dallas, TX, November 1999.
86. Nanotube '99, Michigan State University, Lansing, MI, July 1999 (poster).
87. Joint US/German Workshop on Ultrasensitive Chemistry and Engineering, New Orleans, LA, August 1999 (2 posters).
88. ACS Surfaces and Colloids Symposium (2 presentations), MIT, Boston, MA, June 1999
89. American Conference on Theoretical Chemistry (poster), Boulder, CO, July 1999.
90. Colloids, Polymers and Surfaces Program Mini-symposium, Carnegie Mellon University, Pittsburgh, PA, May 1999.
91. 1999 Midwest Thermodynamics and Statistical Mechanics Conference (2 presentations), Detroit, MI, May 1999
92. Zeolite Membrane Research Group, Chemical Engineering Department, University of Colorado, Boulder, CO, May 1999
93. MRS Fall Meeting, Boston, MA, December 1998.
94. AIChE National Meeting (2 presentations), Miami, FL, November 1998
95. AVS National Symposium, Baltimore, MD, November 1998
96. ACS Surfaces and Colloids Symposium, State College, PA, June 1998.
97. 1998 Midwest Thermodynamics and Statistical Mechanics Conference, Notre Dame, IN, May 1998.
98. AIChE National Meeting, Los Angeles, CA, November 1997 (2 presentations).
99. Materials Science in Chemical Engineering seminar, Department of Chemical Engineering, Pennsylvania State University, State College, PA, January 1997.

100. AIChE National Meeting, Chicago, IL, November 1996 (2 presentations)
101. AVS National Symposium, Philadelphia, PA, October 1996.
102. Surface Science seminar, Department of Physics, University of Maryland, College Park, MD, May 1996.
103. APS March Meeting, St Louis, MO, March 1996.
104. Surface Science seminar, Departments of Chemical Engineering and Chemistry, University of California, Santa Barbara, CA, December 1995.
105. Surface Science seminar, Sandia National Laboratory, Albuquerque, NM, August 1995.
106. Kamp Chaos, Lake Arrowhead, CA, May 1995.
107. Graduate Student Seminar, Program in Applied Mathematics, University of Colorado, Boulder, CO, February 1995.
108. Minisymposium on Phase Transitions in Catalytic Surface Reaction Models, University of Minnesota, Minneapolis, MN, June 1994.
109. Kamp Chaos, Lake Arrowhead, CA, May 1994.
110. Center for Nonlinear Studies, Los Alamos National Laboratory, May 1994.
111. Nonlinear Dynamics seminar, Applied Mathematics Department, University of New South Wales, Sydney, NSW, Australia, December 1993.
112. Chemical Physics After Dark, University of Colorado, Boulder, CO, November 1993.
113. 6th Annual Copper Mountain Conference on Multigrid Methods, Copper Mountain, CO, April 1993.
114. Los Alamos Days at Boulder, Program in Applied Mathematics, University of Colorado, Boulder, CO, March 1993 (poster).

Recognition of Work in Scientific and Popular Press

1. "Taking the heat off distillation", Chemical & Engineering News June 19, 2017
2. Georgia Tech ChBE seminar "The Secrets of Memorably Bad Presentations" covered by Retraction Watch and Chemical and Engineering News, 2017.
3. April 2016 Comment Article in *Nature* by Sholl and Lively covered by outlets including Scientific American, Phys.org, ChemEurope.com, Chem.info.
4. "Supercomputing has a future in clean energy", *Physics Today*, July 2011, 27-28.
5. "Call for Clean Energy Innovation", *Chemical & Engineering News*, June 13, 2011, 29-31
6. "Risky energy research faces uncertain future", *Nature*, March 10 2011, p. 145-146.
7. "Chemical Processing With One Hand", *Chemical Engineering Progress*, October 2009, p.16.
8. Phys. Chem. Chem. Phys. **9** (2007) 1438-1452 featured as an "Editor's Choice" paper in *Science*, March 23, 2007 and highlighted as a "2007 chemistry breakthrough" in *Chemistry World*, December 18, 2007.
9. "Filling Up On Hydrogen", *Chemical and Engineering News*, August 22, 2005 (cover story).
10. "Taking The Pulse Of Catalysis Funding", *Chemical and Engineering News*, November 17, 2003.
11. "Carbon Nanotubes Show Promise as Gas Separation Membranes", *Chemical Engineering Progress*, December 2002.

12. “Nanotubes Could Reduce CO₂ Emissions”, *United Press International*, September 9, 2002. This story was subsequently reprinted in smalltimes.com, Design News and other online outlets.
13. “Chiral Surface Chemistry”, *Chemical and Engineering News*, March 25, 2002 (cover story).
14. “A Hydrogen Filter From Nanotubes”, *Physical Review Focus*, February 1, 1999.

Other Public Products

1. “The Secrets of Memorably Bad Presentations”, Georgia Tech ChBE seminar, Fall 2016, <https://www.youtube.com/watch?v=Bh2bK6zIPdU>
2. “Defects in Metal-Organic Frameworks – Challenge or Opportunity?”, Music video supporting publication in *Journal of Physical Chemistry Letters*, September 2015, <https://www.youtube.com/watch?v=1BS2oKeE9aM>
3. “How to Win the Nobel Prize and Change the World”, Georgia Tech ChBE seminar, Fall 2013, <https://www.youtube.com/watch?v=csRGjRukZpE>

Grants Awarded

1. ExxonMobil Research and Engineering, “Computational Modeling of Specific Interactions of Non-hydrocarbon species”, \$114,000, 11/1/18-11/1/19
2. Department of Energy Advanced Manufacturing Office, “NNMI/RAPID – Focus Area Leader”, \$200,000, 4/1/17-12/31/20 (subcontract from AIChE)
3. Department of Energy Advanced Manufacturing Office, “NNMI/RAPID – A Validated Database of Experimental Adsorption Data”, \$579,000, 1/1/18-12/31/19 (subcontract from AIChE) (Sholl is PI, K. Walton is co-PI) (\$350,000 to Sholl group)
4. Sandia National Laboratory, “Engineered Materials for Deactivation of Chemical Agents”, \$118,000, 10/1/17-9/30/19
5. ExxonMobil Research and Engineering, “Quantitative Predictions of Diffusion in Zeolites”, \$434,000, 4/16/16-4/15/19
6. ExxonMobil Upstream Research, “Modeling Adsorption of Polar Molecules in Complex Adsorbents”, \$548,000, 10/16/15-10/15/19
7. ExxonMobil Research and Engineering, “Modeling Molecular Transport of Gas and Liquid Mixtures in Microporous Materials”, \$339,000, 9/6/16-9/14/19
8. National Science Foundation, “Identifying Upper Bounds for Diffusion-based Separations Using Metal Organic Frameworks”, \$306,042 (\$150,000 to Sholl group), 8/15/16-7/31/19 (Sholl is PI, S. Nair is co-PI)
9. Dow Chemicals, “Recovery of ethylene from dilute reactor effluent streams”, \$1,598,196 (\$380,000 to Sholl group), 10/1/15-9/30/19 (Sholl is PI, K. Walton, R. Lively, M. Realff and Y. Kawajiri are co-PIs)
10. National Science Foundation, “DMREF: Accelerating the discovery and development of nanoporous 2D materials (N2DMs) and membranes for advanced separations”, \$998,543 (\$360,000 to Sholl group), 8/1/15-7/30/18 (S. Nair is PI, D. Sholl, C. Jones and S. Kalidindi are co-PIs)
11. Savannah River National Laboratory, “Multicomponent gas adsorption in nanoporous materials”, \$160,000, 8/1/15-7/30/17 (K. Walton is PI, D. Sholl is co-PI)
12. Department of Energy – NETL, “Enabling 10 mol/kg swing capacity via heat integrated sub-ambient pressure swing adsorption”, \$1,988,714 (\$450,000 to Sholl)

- group), 10/1/15-6/30/19 (R. Lively is PI, D. Sholl, K. Walton, Y. Kawajiri, and M. Realf are co-PIs)
13. ExxonMobil Chemical Co., “Metal-organic frameworks for adsorption-based hydrocarbon separations”, \$532,150 (\$266,075 to Sholl group), 12/1/14-11/30/16 (Sholl is PI, S. Nair and K. Walton are co-PIs)
 14. Oak Ridge National Laboratory, “GO Project: Discovery, Understanding and Validation of Layered Materials”, \$110,000, 5/1/14-4/30/16
 15. Oak Ridge National Laboratory, “GO Project: Layered Ferroics”, \$110,000, 9/1/14-8/30/16
 16. TDA Research/Department of Energy, “Advanced Materials for Personal and Collective Protective Systems”, \$600,000 (\$50,000 to Sholl group), 12/1/13-11/30/15 (K. Walton is PI, Sholl is co-PI)
 17. Department of Energy Energy Frontier Research Center “Center for Understanding and Control of Acid-Gas-Induced Evolution of Materials for Energy (UNCAGE-ME)”, \$18,600,000 (\$974,00 to Sholl group), 8/1/14-7/31/22 (Walton is PI, Sholl is one of 17 co-PIs and Center Deputy Director)
 18. National Science Foundation, “SusChEM: A novel route to an important monomer, 2,5-furandicarboxylic acid, using carbon dioxide captured from air”, \$913,884, 1/1/14-12/31/16, (Jones is PI, Sholl and Bommarius are co-PIs).
 19. Department of Energy Basic Energy Sciences, “Nanoporous Materials Genome Center”, \$820,000 (GT share), 11/12-8/21 (I. Siepmann [U. Minnesota] is PI, Sholl is one of ~10 co-PIs)
 20. National Science Foundation, “Metal Organic Frameworks for efficient separations of liquid mixtures”, \$316,711, 7/13-6/16 (Sholl is PI, Nair is co-PIs)
 21. Phillips66, “Advanced Materials and Membranes for Gas Separations”, \$900,000, 10-12-9/15 (Nair is PI, Sholl and Jones are co-PIs)
 22. ExxonMobil Chemicals, “Recovery of olefins from naphtha using MOFs”, \$342,000, 11/12-10/14 (Sholl is PI, Nair is co-PI)
 23. ExxonMobil Chemicals, “Identification of MOFs for xylene enrichment”, \$378,000, 10/12-9/14 (Sholl is PI, Nair is co-PI)
 24. Dow Chemical, “Membrane reactors for hydrocarbon processing”, \$2,000,000, 10/10-9/14 (Nair is PI, Jones and Sholl are co-PIs)
 25. GE Environmental Services, “Advanced membrane platforms for gaseous fuel conditioning”, \$506,691, 9/11-8/12 (Sholl is PI, Koros, Nair, and Jones are co-PIs)
 26. Department of Energy NETL, “Rapid temperature swing adsorption using polymeric/supported amines”, 11/11-10/14, \$2,200,000 (Jones is PI, Sholl is one of 4 co-PIs)
 27. Department of Energy ARPA-E, “High performance MOF/polymer composite membranes for carbon dioxide capture”, \$1,000,000, 6/10-5/12 (Sholl is PI, Walton, Meredith, Jones, Nair, and Koros are co-PIs)
 28. ExxonMobil Research and Engineering, “Zeolites for Advanced Separations”, \$700,000, 8/10-9/13 (Sholl is PI for 4 task orders, Nair is co-PI on 1 task order)
 29. National Science Foundation, “Unlocking the potential of MOFs as membranes using coupled modeling and experiments”, \$300,000, 7/10-6/13 (Sholl is PI, Nair and Hesketh are co-PIs)

30. Sandia National Laboratory, “Computational modeling of nanoporous framework materials”, \$240,000, 3/10-8/13
31. National Energy Technology Laboratory, “High performance sorbents for carbon dioxide capture from air” \$300,000 12/09-11/12 (Jones (GT) is co-PI, Sholl is PI)
32. National Science Foundation, “High throughput structure sensitive surface chemistry” \$150,000 (GT share) (Sholl and Sykes (Tufts U.) are co-PIs, Gellman (CMU) is PI), 9/10-8/13
33. Department of Energy, Office of Science, “Novel methods of tritium sequestration: high temperature gettering and separation membrane materials discovery for nuclear energy systems”, \$450,000 (GT share) (Sholl and Brinkmann (SRNL) are co-PIs, Chen (U. South Carolina) is PI),
34. National Energy Technology Laboratory, “Amorphous alloy membranes for high temperature hydrogen separations”, \$450,000 (GT share) (Sholl is co-PI, Coulter (SWRI) is PI), 11/09-11/12.
35. Department of Energy Basic Energy Sciences, “Molecular-level Design of Heterogeneous Chiral Catalysis”, \$850,000 (GT share), 11/06-10/12 (Sholl, Tysoe (University of Wisconsin Milwaukee) and Zaera (UC-Riverside) are co-PIs, Gellman (CMU) is PI)
36. Dow Corporation, “Ethanol, Propanol and other high alcohol synthesis from H₂/CO, a combined experimental and computational approach”, \$1,184,000 (C. Jones is PI, Sholl is one of 2 co-PIs), 9/08-8/11
37. ConocoPhillips Corporation, “Advanced Materials and Membranes for Gas Separations”, \$2,376,656 (S. Nair is PI, Sholl is one of 4 co-PIs), 1/09-6/12
38. Department of Energy Basic Energy Science EFRC program, “Catalysis by design – combining experiments and theory for energy applications”, \$800,000 (GT share) (J. Spivey (LSU) is PI, Sholl is one of 12 co-PIs and other senior personnel), 9/09-8/13
39. Department of Energy, Office of Basic Energy Sciences, “Ab initio screening of alloys for hydrogen purification membranes”, \$450,000, 8/08-7/11.
40. Georgia Tech Creating Energy Options Program, “Amorphous Metal Alloys for Hydrogen Purification Membranes”, \$38,500, 7/08-6/09
41. National Science Foundation, “The transition state in catalysis: experiment and computational modeling”, \$494,743, 4/07-2/10 (A. Gellman, PI; Sholl co-PI).
42. National Science Foundation, “NIRT: Gated Transport Through Carbon Nanotube Membranes”, \$200,000 (GT share), 8/07-7/11 (C. Grigoropoulos (Berkeley) is PI, Bakajin (LLNL) and Sholl are co-PIs).
43. National Science Foundation, “Collaborative research: On the structure of naturally chiral metal surfaces”, \$240,000 (CMU and GT share), 7/07-6/10 (C. Sykes (Tufts) is PI, Sholl and Gellman (CMU) are PIs).
44. National Energy Technology Laboratory, “Development of ternary metal alloys for hydrogen purification membranes”, \$300,000 (GT share), 6/07-4/10, (K. Coulter (Southwest Research Institute) is PI, Sholl, and D. Way (Colorado School of Mines) are co-PIs).
45. Pennsylvania Infrastructure Technology Alliance, “Spectroscopic Characteristics of Nanostructured Chiral Surfaces”, \$44,000, 9/06-5/08 (A. Gellman, PI; Sholl co-PI).
46. National Energy Technology Laboratory, “University Computational Materials Consortium”, \$320,000, 1/06-1/07 (Sholl is PI, M. Mavrikakis (U. Wisconsin), M.

- Neurock (U. Virginia), W. Schneider (U. Notre Dame), and J. Li (Ohio State) are co-PIs). ExxonMobil added \$80,000 in matching funding to this grant.
47. Department of Energy Catalysis Futures Program, “Molecular-level Design of Heterogeneous Chiral Catalysis”, \$900,000 (CMU share), 11/06-10/09 (Sholl, Gellman and Tysoe (University of Wisconsin Milwaukee) are co-PIs, Zaera (UC-Riverside) is PI).
 48. National Science Foundation, “GOALI: Multicomponent diffusion in zeolites”, \$320,000, 8/06-7/011 (D. Ruthven (U. Maine) is PI, Sholl and R. Chance (ExxonMobil) are co-PIs).
 49. National Energy Technology Laboratory, “Design and testing of multi-contaminant sorbent materials”, \$262,000, 6/06-5/05 (J. K. Johnson (U. Pittsburgh) is PI, Sholl and R. Parker (U. Pittsburgh) are co-PIs).
 50. Department of Energy, Basic Energy Sciences, “Rapid ab initio screening of ternary alloys for hydrogen purification”, \$300,000, 7/05-6/08.
 51. Department of Energy, “First principles quantum chemistry approaches to predicting surface segregation in metal alloy hydrogen membranes”, \$50,000, 9/05-8/06.
 52. Sandia National Laboratory, “Atomically detailed simulations of molecular mixtures in cationic zeolites”, \$20,000, 5/05-9/05.
 53. Merck Company Foundation, “Separation of Chiral Compounds Using Chiral Surfaces”, \$90,000, 8/04-7/07.
 54. National Science Foundation, “A Combined Theoretical and Experimental Study of Transport of Molecular Mixtures in Zeolite Membranes”, \$433,605 (Sholl is PI, Falconer and Noble (U. Colorado) are co-PIs), 5/04-4/07.
 55. Department of Energy, “Theoretical Studies of Hydrogen Storage in Metal Hydrides”, \$1,250,000 (Sholl is co-PI, Johnson (U. Pittsburgh) is PI), 10/04-5/08. This grant was part of a Metal Hydride Center of Excellence lead by Sandia National Laboratory.
 56. National Science Foundation, “NER: Carbon Nanotube/Polymer Composites for High Flux/High Selectivity Gas Separations”, \$140,000 (Sholl is co-PI, Marand (Virginia Tech.) is PI), 6/04-5/05.
 57. Sandia National Laboratory, “Atomically-detailed simulations of mixture adsorption in zeolites”, \$30,000, 3/04-9/04.
 58. Department of Energy Catalysis Futures Program, “Molecular-level Design of Heterogeneous Chiral Catalysis”, \$800,000 (CMU share), 9/03-11/06 (Sholl, Gellman and Tysoe (University of Wisconsin Milwaukee) are co-PIs, Zaera (UC-Riverside) is PI).
 59. Pennsylvania Infrastructure Technology Alliance, “Computational Thermochemistry of GaAs Contaminants”, \$5,500, 11/03-1/04. (Sholl is PI, D. Yaron is co-PI.)
 60. ACS Petroleum Research Fund, “Density Functional Theory and Lattice Gas Models of Hydrogen Diffusion in CuPd Alloys”, \$80,000, 5/03-8/05.
 61. National Science Foundation, “Catalysis and Separations With One Hand”, \$320,000 (Sholl is PI, A. Gellman is co-PI), 9/02-9/05.
 62. Department of Energy, “EMSP 2002: Transport, Targeting, and Applications of Functional Nanoparticles for Degradation of Chlorinated Organic Solvents”, \$850,000 (G. Lowry is PI, Sholl is one of 4 co-PIs), 9/02-9/05.
 63. ACS Petroleum Research Fund, “Chiral Surfaces Symposium”, \$3,600, 3/03-8/03 (on behalf of the ACS Colloids and Surfaces Division).

64. Department of Energy University Coal Research Program, “Ab-initio studies of Coke Formation on Ni Catalysts During Methane Reforming”, \$197,779, 9/02-1/06.
65. National Science Foundation, “2002 Midwest Thermodynamics and Statistical Mechanics Meeting, May 13-14, 2002, Pittsburgh, PA”, \$6400, 5/02-5/03.
66. Camille Dreyfus Teacher-Scholar Award, \$60,000, 2002.
67. E. Kears Pollock/PPG Industries Grant for Young Faculty, \$100,000, 2002-2005.
68. Pennsylvania Infrastructure Technology Alliance Year 5, “Computational Studies of Chemical Corrosion”, \$39,997, 11/01-12/02. (Sholl is PI, M. Widom is co-PI.)
69. National Energy Technology Laboratory, Department of Energy, “Engineering Support for the Study of Chemisorption and Reactions on Metal Surfaces”, \$57,427, 4/01-8/02.
70. Sloan Foundation Fellowship, \$40,000, 6/01-5/03.
71. National Science Foundation, “Computational Chemical Engineering on a Dedicated Beowulf Cluster”, \$48,330, 3/01-3/02 (Sholl is PI, L. Biegler and S. Hauan are co-PIs).
72. Pennsylvania Infrastructure Technology Alliance Year 4, “Computational Studies of Chemical Corrosion”, \$45,372, 9/00-12/01. (Sholl is PI, M. Widom is co-PI.)
73. National Energy Technology Laboratory, Department of Energy, “Computational Screening of Zeolites for CO₂ Sequestration”, \$157,402, 3/01-3/03.
74. National Energy Technology Laboratory, Department of Energy, “University/NETL Student Partnership”, \$30,000, 9/00-8/01.
75. National Science Foundation, “Carnegie Mellon University Materials Science Engineering and Research Center”, \$4,300,000, 7/01-6/05 (G. Rohrer is PI, Sholl is one of 16 co-PIs).
76. Air Products and Chemicals Inc., “Fundamental Studies of Molecular Diffusion in Zeolite Cavities”, \$15,000, 9/00-8/01.
77. Air Products and Chemicals Inc., “Corrosion of Metal Surfaces by Metal Dusting”, \$25,000, 9/00-9/01.
78. National Science Foundation CAREER Award, “Atomically Detailed Modeling of Transport Through Zeolite Membranes”, \$215,000, 4/00-3/04
79. American Chemical Society Petroleum Research Fund, “Microscopic Characterization of Adsorption and Transport in Aluminophosphate Molecular Sieves”, \$20,000, 9/98-8/00.
80. Carnegie Mellon Faculty Development Fund, “Rational Design of Microporous Membranes using Zeolites and Pore-forming Proteins”, \$5,814, 4/98-4/99.
81. National Science Foundation, "Catalysis With One Hand", \$315,000 (Sholl is PI, A. Gellman is co-PI), 6/99-5/02.
82. National Science Foundation, “Morphological Instability in CdTe Homoepitaxy”, \$100,000 (P. Sides is PI, Sholl is co-PI), 7/99-6/00.
83. Carnegie Mellon Interdisciplinary Course Development Fund, "Development of an Interdisciplinary Course on Molecular Simulations, \$7,500, 7/99-5/00.

Professional Activities

Journal editing:

- Senior editor, *Langmuir*, 2009- (~300 manuscripts per year)
- Member of Elsevier Engineering and Technology Advisory Board, 2008-2010

- Member of Editorial Advisory Board, *Langmuir*, 2008-2009
- Guest editor (with A. Gellman) of special issue of *Journal of Molecular Catalysis A: Chemical* titled “Heterogeneous Chiral Catalysis” Vol. 228 Issues 1-2, 2005
- Guest editor of special issue of *Catalysis Today* titled “Modeling of Catalysis”, Vol. 105, Issue 1, 2005.

Professional Societies:

- AIChE Board of Directors, 2019-2021
- ACS National Award Selection Committee, 2017-2019
- Chair, Computational Molecular Science and Engineering Forum, AIChE, 2012-2014
- Vice-chair, Computational Molecular Science and Engineering Forum, AIChE, 2010-2012
- Area 1a Programming Committee Member, AIChE, 2001-2007

Advisory Boards:

- Department of Chemical Engineering, University of Texas, Austin (2013-2016)
- Department of Chemical Engineering, The Pennsylvania State University, State College, PA (2014-2019)
- Department of Chemical & Biological Engineering, Johns Hopkins University, Baltimore, MD (2016-present)

Journal and Proposal Reviewing: Physical Review Letters, Physical Review B, Chemical Engineering Journal, Journal of Chemical Physics, AIChE Journal, Industrial and Engineering Chemistry Research, Journal of Computational Physics, Physical Review A, Journal of the American Chemical Society, Europhysics Letters, Journal of Physical Chemistry B, Langmuir, Macromolecules, Molecular Simulation, Journal of Catalysis, Nano Letters, Journal of Nanoscience and Nanotechnology, Colloids and Surfaces A, Physical Review E, Journal of Computational Chemistry, Chemical Engineering Communications, Microporous and Mesoporous Materials, Journal of Molecular Catalysis A, ChemPhysChem, Journal of Membrane Science, Nature Materials, Journal of Crystal Growth, Macromolecular Bioscience, Angewandte Chemie, Fluid Phase Equilibria, Science, Journal of Colloid and Interface Science, Journal of Physics: Condensed Matter, Applied Physics Letters, Catalysis Letters, ACS Nano.

Proposal Reviewing: National Science Foundation, Department of Energy, National Institutes of Health, Petroleum Research Fund, Israel Science Foundation, North Carolina Biotechnology Center, Indiana 21st Century Fund, EPSRC, A-STAR, AFOSR, DOE-BES

Book Proposal Reviewing: Blackwell Publishers, John Wiley & Sons

Other Reviewing Activities: Argonne National Lab Center for Nanoscale Materials Proposal Evaluation Board (2007-2011).

Conference Organization:

Chair, Gordon Conference on Chemical Separations, 2020

Co-chair (with S. Nair), International Conference on Inorganic Membranes, 2016

Chair, Gordon Conference on Nanoporous Materials, August 2015

Vice-Chair, Gordon Conference on Nanoporous Materials, August 2013

Co-organizer (with J. K. Johnson), 2002 Midwest Thermodynamics and Statistical Mechanics Meeting

Conference Sessions Chaired:

Session Chair, Process Intensification Topical Conference, AIChE Spring Meeting, San Antonio, TX (6 sessions of invited talks)

Symposium co-chair, "Hydrogen Storage and Purification", AIChE Annual Meeting, Salt Lake City, UT, November 2010

Symposium co-chair, "Chiral Surfaces", ACS National Meeting, Boston, MA, August 2010

Symposium co-chair, "Computational Materials Design in Chemical Industries", ACS National Meeting, San Francisco, California, September 10-14, 2006

Symposium co-chair, "Chirality and Enantioselectivity at Surfaces", ACS National Meeting, San Francisco, California, September 10-14, 2006

Symposium Chair, "Chiral Surfaces", ACS National Meeting, New Orleans, LA, March 2003.

Session vice chair, "Diffusion in Microporous Materials I" and "Diffusion in Microporous Materials II", 2003 AIChE Annual Meeting

Session vice chair, "Thermodynamics and Transport Properties (Posters)", 2003 AIChE Annual Meeting

Organizing committee member, "2003 International Workshop on Zeolitic and Microporous Membranes

Symposium chair, "Computational Methods for Fuels Science", Fuels Division, 2002 ACS National Meeting

Nottingham Competition Judge, 62nd Physical Electronics Conference, Atlanta, GA, June 2002.

Session vice-chair, "Theory and Simulation on the Mesoscale", 2001 AIChE National Meeting

Session vice-chair, "Fundamentals of Surface Processes", 2001 AIChE National Meeting

Symposium co-organizer, "Simulation and Theory of Surfaces, Interfaces, and Complex Fluids", 2001 ACS Colloids and Surface Science Symposium

Executive committee member, 2001 ACS Colloids and Surface Science Symposium

Session vice-chair, "Theory and Simulation on the Mesoscale", 2000 AIChE National Meeting

Session presider, "Physical Chemistry of Chirality", 2000 ACS National Meeting

Session vice-chair, "New Approaches for Simulating Long Time Phenomena", 1999 AIChE National Meeting

Government Committees

Member, National Academies Study Committee, Research Agenda for a New Era in Separations Science, 2018

Invited presenter, NAS Committee on Reproducibility and Replicability in Science, December 2017

Co-chair, DOE BES Basic Research Needs Workshop on the Energy-Water Nexus, January 2017.

NSF Sponsored Workshop on Separations Research Needs for the 21st Century, University of Colorado, July 2004 – invited participant.
National Research Council Workshop on Novel Approaches to Carbon Management: Capture, Sequestration, and Conversion to Useful Products, Irvine, CA, 2003 – invited participant.
NSF Sponsored Workshop on CO₂ Capture and Sequestration, Tulane University, New Orleans, LA, March 2002 – invited participant

Departmental and University Committees

Departmental Computing Committee (CMU) (1999-2000. Chair 2001,2002)
Department PhD Qualifying Exam Committee (CMU) (1999-2002. Chair 2002. 2006)
Department Graduate Recruiting Committee (CMU) (Chair, 2002-2005)
College representative on university-wide Educational Facilities Committee (CMU) (2001)
College ad-hoc promotion and tenure committee (CMU) (2006)
Departmental IT Committee (GT) (2008-2013)
Departmental Graduate Studies Committee (GT) (2008-2013)
Departmental Faculty Advisory Committee (GT) (2009-2012)
Georgia Tech Strategic Planning Steering Committee (2009-2010)
Departmental Faculty Search Committee, Chair (GT) (2011-2013)
GT Taskforce on Scholarship and Fellowship Funds (GT) (2016-2017)
Chair, Search committee for School Chair of Woodruff School of Mechanical Engineering (GT) (2017-2018)

PhD Committees

Committee member on > 70 PhD theses since 2000.

Ph.D. Graduate Students Supervised

1. Timothy D. Power (Graduated 12/01. Postgraduation employer: Shell)
2. Anastasios Skoulidas (Graduated 5/03. Current employer: Exxon Mobil)
3. Aravind Asthagiri (Graduated 5/2003. Current employer: Associate Professor, Ohio State University)
4. Preeti Kamakoti (Graduated 5/05. Postgraduation employer: ExxonMobil)
5. Chong Shang-Shan [Department of Physics] (Graduated 6/05)
6. Rees Rankin (Graduated 5/06. Postgraduation employer: University of Pittsburgh)
7. David Newsome (Graduated 5/06. Postgraduation employer: TUDelft)
8. Bhawna Bhatia (Graduated 9/06. Postgraduation employer: Intel)
9. Haibin Chen (Graduated 8/07. Postgraduation employer: Carbozyme)
10. Xin Li [Department of Chemistry] (Graduated 1/07)
11. Sudhakar Alapati (Graduated 8/07. Postgraduation employer: Intel)
12. Joanna James (Graduated 7/2008. Postgraduation employer: Air Products and Chemicals)
13. Lymarie Semidey-Flecha (Graduated 7/2009. Postgraduation employer: ORNL)
14. Chen Ling (Graduated 12/2009. Postgraduation employer: University of Michigan)
15. Seda Keskin (Graduated 12/2009. Postgraduation employer: Koc University)

16. Sang Eun Jee (Graduated 5/2010. Postgraduation employer: Carnegie Mellon University)
17. Jeong Woo Han (Graduated 5/2010. Postgraduation employer: MIT)
18. Ki Chul Kim (Graduated 8/2010. Postgraduation employer: Northwestern University)
19. Mohamad Kassae [co-advised with Sankar Nair] (Graduated 8/2012. Postgraduation employer: Georgia Tech)
20. Emmanuel Haldoupis (Graduated 5/2013. Postgraduation employer: University of Minnesota)
21. Sung Gu Kang (Graduated 5/2013. Postgraduation employer: Cornell University)
22. Liwei Li (Graduated 5/2014. Postgraduation employer: Dow Chemical Company)
23. Nita Chandrasekhar (Graduated 5/2014. Postgraduation employer: Praxair)
24. Dieh Teng (Graduated 5/2014. Postgraduation employer: KBR)
25. Ambarish Kulkarni (Graduated: 12/2014. Postgraduation employer: Stanford University)
26. Kelly Nicholson (Graduated 8/2014. Postgraduation employer: Praxair)
27. Daniel Wei (Graduated 12/2014)
28. Jason Gee (Graduated 8/2015. Postgraduation employer: ExxonMobil)
29. Ben Chun [co-advised with Seung Sung Jang] (Graduated 5/2015)
30. Rohan Awati (Graduated 12/2015) [Georgia Tech]
31. Hakan Demir (Graduated 5/2016) [University of Minnesota]
32. Seung Won Choi [co-advised with Sankar Nair and Chris Jones] (Graduated 5/2016) [LG Chemicals]
33. Jeffrey Camp (Graduated 5/2016) [LLBL]
34. Ross Verploegh (Graduated 8/2017) [GT]
35. Dalar Nazarian (Graduated 8/2016) [Praxair]
36. Lalit Darunte [co-advised with Krista Walton and Chris Jones] (Graduated 5/2018) [Dow Chemicals]
37. Jungseob So [co-advised with Carsten Sievers] (Graduated 5/2018) [Samsung]
38. Yang Liu (Graduated 12/2018) [Dow Chemical]
39. Chu Han (Graduated 12/2018)
40. Souryadeep Bhattacharyya [co-advised with Sankar Nair] (Graduated 12/2018) [GT]
41. Rebecca Han (expected graduation: 5/2019)
42. Mayank Agrawal (expected graduation: 5/2019)
43. Jongwoo Park (expected graduation: 5/2020)
44. Omar Knio (expected graduation: 5/2020)
45. John Findley (expected graduation: 5/2019)
46. Wenqin You (expected graduation: 5/2020)
47. Andrew Chen (expected graduation: 5/2021)
48. Zhenzi Yu (expected graduation: 5/2022)
49. Yuhang Yang (expected graduation: 5/2022)
50. Alan Daou (expected graduation: 5/2022)
51. Arvind Ganesan [co-advised with Sankar Nair] (expected graduation: 5/2022)

M.S. Graduate Students Supervised

1. David Blanco-Maceiras (Graduated 5/02. Postgraduation employer, BOC)
2. Namory Keita (Graduated 5/12)

3. Timothy van Heest (Graduated 5/12)
4. Alex Fergusson (Graduated 5/12)
5. Kenechukwu Onubugo [co-advised with Krista Walton] (Graduated 5/14)
6. Charles Pueschel (Graduated 12/15)
7. Brandon Plaisance (Graduated 5/16)
8. Xuqing Cai (expected graduation: 5/20)

Undergraduate Students Supervised [Postgraduate placement if known]

Vikram Gopal (1/17-)
 Adithya Krishnachand (1/17-)
 Marija Milansovic (6/15-5/16)
 Samuel Swanson (9/11-6/12)
 Philip Miller (9/11-12/11)
 Benjamin Ivey (9/11-5/12)
 Victor Manrique (9/10-5/11)
 Madison Barre (9/10-5/11)
 Estelle Kinnaird (9/10-5/11)
 Megan DeWitt (9/10-5/11)
 Christopher Kim (5/10-5/11)
 Courtney Brown (9/09-5/10, 8/10-5/11)
 Allan Choi (5/09-5/11)
 Michael Reid Davis (5/09-5/10)
 Darshan Mithaiwala (1/09-12/09)
 Jesse McBride (1/09-12/10)
 Michael Jones (1/09-5/10)
 Angela Dapolite (6/07-8/07)
 Jacqui Tehranchi (9/04-8/05)
 Kenneth Hu (9/04-8/05)
 Adam Edison (9/04-5/05)
 Jennifer Njoroge (9/04-5/05)
 Asako Hayashi (9/04-5/05)
 Adam Welander (9/03-5/04) [Graduate student at U. Wisconsin]
 Felix Yip (1/03-5/04)
 Daniel Caballero (1/02-8/02) [Graduate student at Illinois Institute of Technology]
 Kurt Ken Sieber (3/02-12/03)
 Amy K. Lin (9/00-5/01) [ExxonMobil]
 Preeti Kamakoti (6/00-8/00) [Graduate student at CMU]
 Stephen Cisar (9/99 - 5/00) [Graduate student at Northwestern University]
 Daniel Sheehan (9/99 – 5/00)
 Michael K. Fenwick 9/98-8/99 [Graduate student at Cornell]
 David R. Dunsavage, 9/98-5/99 [Westinghouse]
 Cha Kun Lee, 9/98-5/99 [Graduate student at MIT]

High School Students Supervised

Long Dinh (10/09-4/10, 10/10-5/11)

Awards to Supervised Graduate and Undergraduate Students

Seda Keskin, Sigma Xi Best Thesis Award, Georgia Institute of Technology, 2009
Lymarie Semidey-Flecha, Goizueta Fellowship, Georgia Institute of Technology, 2008.
Lymarie Semidey-Flecha, Student presentation award, Pittsburgh Cleveland Catalysis Society Spring meeting, 2007.
Sudhakar Alapati, Ken Meyer Memorial Award for Excellence in Graduate Research, CMU Department of Chemical Engineering, 2007.
Lymarie Semidey-Flecha, Gordon Conference Travel award, 2006.
Rees Rankin, Student presentation award, Pittsburgh Cleveland Catalysis Society Spring meeting, 2006.
Preeti Kamakoti, Ken Meyer Memorial Award for Excellence in Graduate Research, CMU Department of Chemical Engineering, 2005.
Joanna James, Bayer Graduate Fellowship, CMU Department of Chemical Engineering, 2005-2008.
Preeti Kamakoti, 3rd prize, Student paper contest, 8th International Conference on Inorganic Membranes, Cincinnati, OH, July 2004
Preeti Kamakoti, Symposium Award, CHEGSA symposium, 2004
Bhawna Bhatia, Poster award, CHEGSA symposium, 2003
Anastasios Skoulidas, AIChE Separations Division Graduate Student Award in Membrane-Based Separations, 2002.
Aravind Asthagiri, Division of Chemical Physics Travel Award, American Physical Society, 2002.
Timothy D. Power, Geoffrey D. Parfitt Memorial Award, CHEGSA Symposium, 2001
Aravind Asthagiri, Honorable Mention, CHEGSA Symposium, 2001
Anastasios Skoulidas, Gordon Conference Travel Award, 2001
Amy K. Lin, 2nd Place Winner in CIT Honors Program poster session, 2001
Timothy D. Power, Honorable Mention, CHEGSA Symposium, 2001
Aravind Asthagiri, Symposium Award, CHEGSA Symposium, 2000
Michael K. Fenwick, 2nd Place Winner in CIT Honors Program Poster session, 1999
Timothy D. Power, Symposium Award, CHEGSA Symposium, 1999

Postdoctoral Researchers Supervised

1. Dr. Tao Li, 8/01-9/02
2. Dr. Vaishali Shah, 3/01-3/03
3. Dr. E. Demet Akten, 1/01-10/02
4. Dr. Abdulwahab Almusallam, 10/02-6/05
5. Dr. Shiqiang Hao, 8/06-10/11
6. Dr. Pawel Szabelski (Fulbright Fellow), 8/06-12/06
7. Dr. Ji Zang, 1/08-10/12
8. Dr. Taku Watanabe, 6/08-6/12
9. Dr. Thomas Manz, 10/08-7/12
10. Dr. Xuerong Shi, 11/10-10/12
11. Dr. Hanjun Fang, 12/10-
12. Dr. Iyad Hijazi, 1/11-1/12
13. Dr. Salah Boulfelfel, 6/12-
14. Dr. Veronika Walkosz, 8/12-9/13
15. Dr. Rongshun Zhu, 9/12-10/14

16. Dr. Melissa Lucero, 11/12-3/14
17. Dr. Xiaowa Nie, 8/14-1/15
18. Dr. Joshua Howe, 11/14-7/18
19. Dr. Dai Tang, 1/16-
20. Dr. Rohan Awati, 9/16-10/18
21. Dr. Alex Hyla, 1/17-12/17
22. Dr. Anh Pham, 1/18-5/18
23. Dr. Farhad Gharagheizi, 6/18-
24. Dr. Raghuram Thyagarajan, 8/18-
25. Dr. Jifeng Sun, 11/18-