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

7/21 – present, Director, Transformational Decarbonization Initiative, Oak Ridge National Laboratory, Oak Ridge, TN
7/21 – present, Professor, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA
10/16 – 6/21, 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. Portfolio Strategy Advisor, Department of Energy Office of Clean Energy Demonstrations (OCED), 2022-2023
2. Editor-in-chief, *AIChE Journal*, 2022-present

3. Panel member, National Academies Study Committee, Chemical Engineering: Challenges and Opportunities in the 21st Century, 2020-2021
4. Panel lead, DOE BES Basic Research Needs Workshop on Transformative Manufacturing, 2020
5. Board of Directors, American Institute of Chemical Engineers, 2019-2021
6. Chair, Inaugural Gordon Conference on Chemical Separations, 2020
7. Organizing Committee, Chemical Engineering National Diversity Equity Workshop, 2021
8. Panel member, National Academies Study Committee, Research Agenda for a New Era in Separations Science, 2018-2019
9. Member, AIChE Strategic Plan Steering Committee, 2018
10. Interim Chief Technology Officer (8/16-3/17) and Focus Area Lead (Modeling & Simulation) (3/17-present), RAPID National Manufacturing Institute, AIChE.
11. Co-chair, DOE BES Basic Research Needs Workshop on the Energy-Water Nexus, 2017.
12. School Chair, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, 7/13-6/21.
13. Co-chair, International Conference on Inorganic Membranes 2016.
14. Chair, Gordon Conference on Nanoporous Materials, 8/15.
15. Deputy Director, UNCAGE-ME (DOE Energy Frontier Research Center), 8/14-present.
16. Chair, Computational Molecular Science and Engineering Forum, AIChE, 2012-2014.
17. Co-founder, *InmondoTech Inc*., 2013-2018
18. Associate Director, Strategic Energy Institute, Georgia Institute of Technology, Atlanta, GA, 1/10-6/13.
19. Senior editor, *Langmuir*, 2009-2019.

Awards and Distinctions

1. Kurt Wohl Memorial Lecture, Department of Chemical and Biomolecular Engineering, University of Delaware (2023)
2. Georgia Tech Curriculum Innovation Award [jointly with several faculty from Georgia Tech] (2022)
3. Chemical Engineering Alumni Lectures, University of Massachusetts Amherst (2021)
4. Fellow, American Association for the Advancement of Science (2020)
5. Doumas Lecture in Chemical Engineering, Virginia Tech (2019)
6. Fellow, American Institute of Chemical Engineering (2019)
7. Institute Award for Excellence in Industrial Gases Technology, American Institute of Chemical Engineering (2018)
8. Parr Lecturer, Department of Chemical and Biomolecular Engineering, University of Illinois (2018)
9. "Highly Prolific Author" recognition, Journal of Physical Chemistry C (2017)
10. AIChE Gary Leach Award [jointly with several faculty and staff from Georgia Tech] (2015)
11. Early Career Achievement Award, Computational Molecular Science and Engineering Forum, AIChE (2010)

12. DOE Hydrogen Program R&D Award (2008)
13. MESD Plenary Session speaker, AIChE Annual Meeting (2007)
14. COMSEF Plenary Session speaker, AIChE Annual Meeting (2006)
15. CAST Plenary Session speaker, AIChE Annual Meeting (2002)
16. Camille Dreyfus Teacher-Scholar Award (2002)
17. E. Kears Pollock/PPG Industries Grant for Young Faculty (2002-2005)
18. Alfred P. Sloan fellow (2001-2003)
19. George Tallman Ladd Award for Excellence in Research, Carnegie Institute of Technology, Carnegie Mellon University (2000)
20. National Science Foundation CAREER Award (2000-2004)
21. Faculty Fellow, National Energy Technology Laboratory (2000-2007)
22. APS Division of Chemical Physics Travel Award (1996).
23. University of Colorado Graduate School Research and Creative Work Award (1995).
24. Honorable mention, NSF Graduate Research Fellowship (1991).
25. University of Colorado Doctoral Fellowship (1991).
26. University Medal, Australian National University (1991).
27. Education Abroad Scholar, University of California (1988-1989).
28. National Undergraduate Scholarship, Australian National University (1987-1991).

Research Publications (> 26,000 citations, h-index = 86 as reported by Web of Science)
[Publications with > 50 citations indicated by * and with > 100 citations indicated by **]

1. *Selective uptake of ethane/ethylene mixtures by UTSA-280 is driven by reversibly coordinated water defects,* Yutao Gong, Xuqing Cai, Wenqin You, Xiao Jiang, Wei Liu, Ryan Lively, Krista S. Walton, and David S. Sholl, Chemistry of Materials, 35 (2023) 2956-2966
2. *A membrane contactor enabling energy-efficient CO_2 capture from point sources with deep eutectic solvents,* Syed Z. Islam, Md Arifuzzaman, Gernot Rother, Vera Bocharova, Robert L. Sacci, Jacek Jakowski, Jingsong Huang, Ilia Nicolaevich Ivanov, Ramesh R. Bhave, Tomonori Saito, and David S. Sholl, Industrial & Engineering Chemistry Research, 62 (2023) 4455-4465
3. *Strong degradation of polycarbonate and polystyrene by the CO_2 capture solvent diethyl sebacate,* Syed Z. Islam, David S. Sholl, Janice A. Steckel, and Robert L. Thompson, Process Safety Progress, 42 (2023) 371-376
4. *New data sharing requirements for AIChE Journal authors,* David S. Sholl, AIChE Journal, 69 (2023) e18017
5. *Identifying high-performance metal-organic frameworks for low-temperature oxygen recovery from helium by computational screening,* Shubham Jamdade, Rishi Gurnani, Hanjun Fang, Salah Eddine Boulfelfel, Rampi Ramprasad, and David S. Sholl, Industrial & Engineering Chemistry Research, 62 (2023) 1927-1935
6. *Development of porous crystalline materials for selective binding of O_2 from air,* Jifeng Sun, Farhad Gharagheizi, Hanjun Fang, Peter I. Ravikovitch, and David S. Sholl, Journal of Physical Chemistry C, 127 (2023) 776-787
7. *Assessment of Acid Gas Adsorption Selectivities in MIL-125-NH_2,* Chunyi Li, Zhenzhi Yu, Kai Cui, J. R. Schmidt, David S. Sholl, and Ryan P. Lively, Journal of Physical Chemistry C, 126 (2022) 21414-21425

8. *Adapting UFF4MOF for heterometallic rare-earth metal-organic frameworks,* Yuhan Yang, Ifayoyinsola A. Ibikunle, Dorina F. Sava Gallis, and David S. Sholl, ACS Applied Materials & Interfaces, 14 (2022) 54101-54110
9. *Trends in siting of metals in heterometallic Nd-Yb metal-organic frameworks and molecular crystals,* Ifayoyinsola A. Ibikunle, Yuhan Yang, Nichole R. Valdez,Mark A. Rodriguez, Jacob A. Harvey, Dorina F. Sava Gallis, and David S. Sholl, ACS Applied Materials & Interfaces, 14 (2022) 54349-54358
10. *Assessment of acid gas adsorption selectivities in MIL-125-NH_2,* Chunyi Li, Zhenzi Yu, Kai Cui, J. R. Schmidt, David S. Sholl and Ryan P. Lively, Journal of Physical Chemistry C, 126 (2022) 21414-21425
11. *Theoretical pathway towards improved reverse osmosis membrane selectivity for neutral solutes: Inspiration from gas separations,* Haley D. White, Hannah G. Huang, Margaret C. D'Amaro, Elisa A. Mignone, David S. Sholl, and Ryan P. Lively, Journal of Physical Chemistry C, 126 (2022) 19496-19506
12. *Unlocking a rigid purine MOF for kinetic separation of xylenes,* Richelle Lyndon, Yuxiang Wang, Ian M. Walton, Yao Ma, Yang Liu, Zhenzi Yu, Guanghui Zhu, Samuel Berens, Yu-Sheng Chen, SuYin Wang, Sergey Vasenkov, David S. Sholl, Krista S. Walton, Simon H. Pang, and Ryan P. Lively, Chemical Communications, 58 (2022) 12305-12308
13. *Achieving order of magnitude increases in CO_2 reduction reaction efficiency by product separations and recycling,* Akriti Sarswat, David S. Sholl, and Ryan P. Lively, Sustainable Energy & Fuels, 6 (2022) 4598-4604
14. *Online graduate certificate in data science for the chemical industry,* Andrew Medford, Fani Boukouvala, Martha Grover, David Sholl, Carson Meredith, Pengfei Cheng, Sihoon Choi, Gabriel Gusmao, Zachary Kilwein, Suryateja Ravutla, Fatimah Wirth, Zaid Sewer, Jennifer Wooley, Chemical Engineering Education, 56 (2022) 249-259
15. *Metal-organic Framework Integrating Framework and Bimetallic Coupling Effect for Highly Efficient Oxygen Evolution Reaction,* Shulin Li, Tienan Wang, Dai Tang, Yuting Yang, Yuyang Tian, Fengchao Cui, Jifeng Sun, Xiaofei Jing, David S. Sholl, and Guangshan Zhu, Advanced Science, 9 (2022) 2203712
16. *Curated Collection of More than 20,000 Experimentally-reported One-Dimensional Metal-Organic Frameworks,* Farhad Gharagheizi, Zhenzi Yu, and David S. Sholl, ACS Applied Materials & Interfaces, 14 (2022) 42258-42266
17. *Point defects control guest diffusion in the 1D pores of Zn(tbip),* Xuqing Cai and David S. Sholl, Journal of Physical Chemistry C, 126 (2022) 14321-14328
18. *Kinetic model of acid gas induced defect propagation in zeolitic imidazolate frameworks,* Kai Cui, Sankar Nair, David S. Sholl, and J. R. Schmidt, Journal pf Physical Chemistry Letters, 13 (2022) 6541-6548
19. *Experimentally verified alkane adsoption isotherms in nanoporous materials from literature meta-analysis,* Lukas W. Bingel, Krista S. Walton, and David S. Sholl, Journal of Chemical and Engineering Data, 67 (2022) 1757-1764
20. *Discrepancy quantification between experimental and simulated data of CO_2 adsorption isotherm using hierarchical Bayesian estimation,* Sotaro Kojima, Jongwoo Park, Eli A. Carter, Krista S. Walton, Matthew J. Realff, David S. Sholl, Tomoyuki

Yajima, Junpei Fujiki and Yoshiaki Kawajiri, Separation and Purification Technology, 296 (2022) 121371

21. *How reproducible are surface areas calculated from the BET equation?* Johannes W. M. Osterrieth, Jarnes Rampersad, David Madden, David S. Sholl, David Fairen-Jiminez et al. [>50 authors in total], Advanced Materials, 34 (2022) 2201502
22. *Gaussian approximation of dispersion potentials for efficient featurization and machine-learning predictions of metal-organic frameworks,* Sihoon Choi, David S. Sholl, and Andrew J. Medford, Journal of Chemical Physics, 156 (2022) 214108
23. *Effect of loading on the water stability of the metal-organic framework DMOF [Zn(bdc)(dabco)$_{0.5}$],* Carmen Chen, Zhenzi Yu, David S. Sholl and Krista S. Walton, Journal of Physical Chemistry Letters, 13 (2022) 4891-4896
24. *Molecular simulations of CH_4 and CO_2 diffusion in rigid amorphous materials,* Raghu Thyagarajan and David S. Sholl, Journal of Physical Chemistry C, 126 (2022) 8530-8538
25. *In silico design of microporous polymers for chemical separations and storage,* Dylan M. Anstine, David S. Sholl, Joern Ilja Siepmann, Randall Q. Snurr, Alán Aspuru-Guzik and Coray M. Colina, Current Opinion in Chemical Engineering, 36 (2022) 100795
26. *Accelerating solvent selection for type II porous liquids,* Chao-Wen Chang, Isaiah Borne, Robin M. Lawler, Zhenzhi Yu, Seung Soon Jang, Ryan P. Lively and David S. Sholl, Journal of the American Chemical Society, 144 (2022) 4071-4079
27. *A systematic examination of the impacts of MOF flexibility on intracrystalline molecules diffusivities,* Yuhan Yang and David S. Sholl, Journal of Materials Chemistry A, 10 (2022) 4242-4253
28. *Exemplar mixtures for studying complex mixture effects in practical chemical separations,* David S. Sholl and Ryan P. Lively, JACS Au, 2 (2022) 322-327
29. *Opening the toolbox: 18 experimental techniques for measurements of mixed gas adsorption,* Danny Shade, Brandon W. S. Bout, David S. Sholl and Krista S. Walton, Industrial & Engineering Chemistry Research 61 (2022) 2367-2391
30. *Single-walled zeolitic nanotubes,* Akshay Korde, Byunghyun Min, Elina Kapaca, Omar Knio, Iman Nezam, Ziyuan Wang, Johannes Leisen, Xinyang Yin, Xueyi Zhang, David S. Sholl, Xiaodong Zou, Tom Wilhammar, Christopher W. Jones and Sankar Nair, Science, 375 (2022) 62
31. *Comprehensive assessment of the accuracy of the Ideal Adsorbed Solution Theory for predicting binary adsorption of gas mixtures in porous materials,* Farhad Gharagheizi and David S. Sholl, Industrial & Engineering Chemistry Research, 61 (2022) 727-739
32. *Incorporating flexibility effects into metal-organic framework adsorption simulations using different models,* Zhenzi Yu, Dylan M. Anstine, Salah Eddine Boulfelfel, Chenkai Gu, Coray M. Colina and David S. Sholl, ACS Applied Materials & Interfaces, 13 (2021) 61305-61315
33. *A transferable force field for predicting adsorption and diffusion of small molecules in alkali exchanged zeolites with coupled cluster accuracy,* Salah Eddine Boulfelfel, John M. Findley, Hanjun Fang, Alan S. S. Daou, Peter I. Ravikovitch and David S. Sholl, Journal of Physical Chemistry C, 125 (2021) 26832-26846

34. *Computational screening of MOFs and zeolites for direct air capture of carbon dioxide under humid conditions,* John M. Findley and David S. Sholl, Journal of Physical Chemistry C, 125 (2021) 24630-24639
35. *Controlled demolition and reconstruction of imidazolate and carboxylate metal-organic frameworks by acid gas exposure and linker treatment,* Arvind Ganesan, Stephen C. Purdy, Zhenzi Yu, Souryadeep Bhattacharyya, Katharine Page, David S. Sholl and Sankar Nair, Industrial & Engineering Chemistry Research, 60 (2021) 15582-15592
36. *High throughput screening of anion-pillared metal-organic frameworks for the separation of light hydrocarbons,* Chenkai Gu, Jing Liu and David S. Sholl, Journal of Physical Chemistry C, 125 (2021) 20076-20086
37. *Analysis of energetics and economics of sub-ambient hybrid post-combustion carbon dioxide capture,* Stephen J. A. DeWitt, Rohan Awati, Hector Octavio Rubiera Landa, Jongwoo Park, Yoshiaki Kawajiri, David S. Sholl, Matthew J. Realff and Ryan P. Lively, AIChE Journal (2021) e17403
38. *Efficient models for predicting temperature-dependent Henry's constants and adsorption selectivities for diverse collections of molecules in metal-organic frameworks,* Xiaohan Yu, Sihoon Choi, Dai Tang, Andrew J. Medford and David S. Sholl, Journal of Physical Chemistry C, 125 (2021) 18046-18057
39. *Fingerprinting diverse nanoporous materials for optimal hydrogen storage conditions using meta-learning,* Yangzesheng Sun, Robert F. DeJaco, Zhao Li, Dai Tang, Stephan Glante, David S. Sholl, Coray M. Colina, Randall Q. Snurr, Matthias Thommes, Martin Hartmann and J. Ilja Siepmann, Science Advances 7 (2021) eabg3983
40. *Interpretable machine learning-based predictions of methane uptake isotherms in metal-organic frameworks,* Rishi Gurnani, Zhenzi Yu, Chiho Kim, David S. Sholl and Rampi Ramprasad, Chemistry of Materials 33 (2021) 3543-3552
41. *A transferable force field for predicting adsorption and diffusion of hydrocarbons and small molecules in silica zeolites with coupled-cluster accuracy,* John M. Findley, Salah Eddine Boulfelfel, Hanjun Fang, Giovanni Muraro, Peter I. Ravikovitch and David S. Sholl, Journal of Physical Chemistry C 125 (2021) 8418-8429
42. *Adsorption space for microporous polymers with diverse adsorbate species,* Dylan M. Anstine, Dai Tang, David S. Sholl and Coray M. Colina, NPJ Computational Materials 7 (2021) 53
43. *Quantifying impact of intrinsic flexibility on molecular adsorption in zeolites,* Alan S. S. Daou, John M. Findley, Hanjun Fang, Salah Eddine Boulfelfel, Peter I. Ravikovitch and David S. Sholl, Journal of Physical Chemistry C 125 (2021) 5926-5305
44. *Construction of an anion-pillared MOF database and the screening of MOFs suitable for Xe/Kr separation,* Chenkai Gu, Zhenzi Yu, Jing Liu and David S. Sholl, ACS Applied Materials and Interfaces 13 (2021) 11039-11049
45. *Adsorption-based separation of near-azeotropic mixtures: a challenging example for high-throughput development of adsorbents,* Dai Tang, Farhard Gharagheizi and David S. Sholl, Journal of Physical Chemistry B 125 (2021) 926

46. *A collection of more the 900 gas mixture adsorption experiments in porous materials from literature meta-analysis,* Xuqing Cai, Farhad Gharagheizi, Lukas W. Bingel, Danny Shade, Krista S. Walton and David S. Sholl, Industrial and Engineering Chemistry Research 60 (2021) 639
47. *First-principles study of electronic and optical properties of ternary compounds $AuBX_2$ (X = S, Se, Te) and $AuMTe_2$ (M = Al, In, Ga),* Muhammad Shahzad Yaseen, Jifeng Sun, Hanjun Fang, G. Murtaza and David S. Sholl, Solid State Sciences 111 (2021) 106508
48. *Spin-crossover effects in reversible O_2 binding on a dinuclear cobalt(II) complex,* Jifeng Sun, Hanjun Fang, Peter I. Ravikovitch and David S. Sholl, Journal of Physical Chemistry C, 124 (2020) 26843-26850 DOI: 10.1021/acs/jpcc.0c08629
49. *In-situ IR spectroscopy study of reactions of C_3 oxygenates on heteroatom (Sn, Mo, and W) doped BEA zeolites and the effect of co-adsorbed water,* Sean Najmi, Jungseob So, Eli Stavitski, William P. McDermott, Yimeng Lyu, Sam P. Burt, Ive Hermans, David S. Sholl and Carsten Sievers, ChemCatChem, DOI: 10.1002/cctc202001424
50. *A database of porous rigid amorphous materials,* Raghuram Thyagarajan and David S. Sholl, Chemistry of Materials, 32 (2020) 8020-8033
51. *Experimentally verified alcohol adsorption isotherms in nanoporous materials from literature meta-analysis,* Lukas W. Bingel, Andrew Chen, Mayank Agrawal and David S. Sholl, Journal of Chemical Engineering Data, 65 (2020) 4970-4979
52. *Tuning the wettability of metal-organic frameworks via defect engineering for efficient oil/water separation,* Yi Huang, Yang Jiao, Ting Chen, Yutao Gong, Songcheng Wang, Liu Yang, David S. Sholl and Krista S. Walton, ACS Applied Materials and Interfaces, 12 (2020) 34413-34422
53. *Molecular dynamics investigation of surface resistances in zeolite nanosheets,* Omar Knio, Hanjun Fang, Salah Eddine Boulfelfel, Sankar Nair and David S. Sholl, Journal of Physical Chemistry C, 124 (2020) 15241-15252
54. *Effect of humidity on the sorption of H_2S from multicomponent acid gas streams on silica-supports sterically hindered and unhindered amines,* Claudia N. Okwonko, Hanjun Fang, David S. Sholl, Johannes E. Leisen and Christopher W. Jones, ACS Sustainable Chemistry & Engineering, 8 (2020) 10102-10114
55. *Using site heterogeneity in metal-organic frameworks with bimetallic open metal sites for olefin/paraffin separations,* Wenqin You, Trisha Sen, Yoshiaki Kawajiri, Matthew J. Realff and David S. Sholl, ACS Applied Nano Materials, 3 (2020) 5291-5300
56. *Tuning the structures of metal-organic frameworks via a mixed-linker strategy for ethylene/ethane kinetic separation,* Richelle Lyndon, Wenqin You, Yao Ma, John Bacsa, Yutao Gong, Eric E. Stangland, Krista S. Walton, David S. Sholl and Ryan P. Lively, Chemistry of Materials, 32 (2020) 3715-3722
57. *How well do approximate models of adsorption-based CO_2 capture processes predict results of detailed process models?* Jongwoo Park, Hector Octavio Rubiera Landa, Yoshiaki Kawajiri, Matthew Realff, Ryan P. Lively and David S. Sholl, Industrial & Engineering Chemistry Research, 59 (2020) 7097-7108
58. *Impact of intrinsic framework flexibility for selective adsorption of sarin in non-aqueous solvents using metal-organic frameworks,* Jongwoo Park, MayankAgrawal,

Dorina F. Sava Gallis, Jacob A. Harvey, Jeffrey A. Greathouse, and David S. Sholl, Physical Chemistry Chemical Physics, 22 (2020) 6441-6448

59. *Hierarchical Bayesian estimation for adsorption isotherm parameter estimation,* Chunkai Shih, Jongwoo Park, David S. Sholl, Matthew J. Realff, Tomoyuki Yajima and Yoshiaki Kawajiri, Chemical Engineering Science, 214 (2020) 115435
60. *Watching Water, Sodium, and Chloride Passing through a Graphitic Pore,* David S. Sholl, Matter, 2 (2020) 524-525
61. *Selecting Adsorbents to Separate Diverse Near-Azeotropic Chemicals,* Farhad Gharagheizi, Dai Tang and David S. Sholl, Journal of Physical Chemistry C, 124 (2020) 3664-3670
62. *A strong test of atomically detailed model of molecular adsorption in zeolites using multilaboratory experimental data for CO_2 adsorption in ammonium ZSM-5,* Hanjun Fang, John Findley, Giovanni Muraro, Peter I. Ravikovitch and David S. Sholl, Journal of Physical Chemistry Letters, 11 (2020) 471-477
63. *Does repeat synthesis in materials chemistry obey a power law?* Mayank Agrawal, Rebecca Han, Dinushka Herath and David S. Sholl, Proceeding of the National Academies of Science, 117 (2020) 877-822
64. *Understanding dealumination mechanisms in protonic and cationic zeolites,* Jifeng Sun, Hanjun Fang, Peter I. Ravikovitch and David S. Sholl, Journal of Physical Chemistry C, 124 (2020) 668-676
65. *Quantitative correlations for the durability of zeolitic imidazolate frameworks in humid SO_2,* Souryadeep Bhattacharyya, David S. Sholl and Sankar Nair, Industrial and Engineering Chemistry Research, 59 (2020) 245-252
66. *Determining diffusion coefficients of chemical warfare agents in metal-organic frameworks,* Mayank Agrawal, Salah E. Boulfelfel, Dorina F. Sava Gallis, Jeffrey A Greathouse and David S. Sholl, Journal of Physical Chemistry Letters, 10 (2019) 7823-7830
67. ***Advances, updates and analytics for the Computation-Ready, Experimental Metal-organic Framework Database: CoRE MOF 2019,* Youngchul G. Chung, Emmanuel Haldoupis, Benjamin J. Bucior, Maciej Haranczyk, Seulchan Lee, Hongda Zhang, Konstantinos D. Vogiatzis, Marija Milisavljevic, Sanliang Ling, Jeffrey S. Camp, Ben Slater, J. Ilja Siepmann, David S. Sholl and Randall Q. Snurr, Journal of Chemical and Engineering Data, 64 (2019) 5985-5998
68. *Five easy ways to make your research more reproducible,* David S. Sholl, Langmuir, 35 (2019) 13257-13258
69. *Synthesizing new hybrid zeolitic imidazolate frameworks by controlled demolition and reconstruction,* Krishna C. Jayachandrababu, Yadong Chiang, Fengyi Zhang, Akshay Korde, Rebecca Han, Souryadeep Bhattacharyya, David S. Sholl and Sankar Nair, ACS Materials Letters 1 (2019) 447-451
70. *In-situ ATR-IR study of surface reaction during aqueous phase reforming of glycerol, sorbitol and glucose over Pt/γ-Al_2O_3,* Jungseob So, Yoona Chung, David S. Sholl, and Carsten Sievers, Molecular Catalysis, 475 (2019) 110423
71. *Effects of intrinsic flexibility on adsorption properties of metal-organic frameworks at dilute and nondilute loadings,* Mayank Agrawal and David S. Sholl, ACS Applied Materials and Interfaces, 11 (2019) 31060-31068

72. *Significant temperature dependence of the isosteric heats of adsorption of gases in zeolites demonstrated by experiments and molecular simulations,* Alexander S. Hyla, Hanjun Fang, Salah Eddine Boulfelfel, Giovanni Muraro, Charanjit Paur, Karl Strohmaier, Peter I. Ravikovitch and David S. Sholl, Journal of Physical Chemistry C, 123 (2019) 20405-20412
73. *Does chemical engineering have a reproducibility problem?* Rebecca Han, Krista S. Walton and David S. Sholl, Annual Review of Chemical and Biomolecular Engineering, 10 (2019) 43-57
74. *Rapid prediction of adsorption isotherms of a diverse range of molecules in hyper-crosslinked polymers,* Dai Tang, Grit Kupgan, Coray M. Colina and David S. Sholl, Journal of Physical Chemistry C, 123 (2019) 17884-17893
75. *Sorption and transport of vapors in ZIF-11: Adsorption, diffusion, and linker flexibility,* Brian R. Pimentel, Melinda L. Jue, Er-Kang Zhou, Ross J. Verploegh, Johannes Leisen, David S. Sholl, and Ryan P. Lively, Journal of Physical Chemistry C, 123 (2019) 12862-12870
76. *Propagation of degradation-induced defects in zeolitic imidazolate frameworks,* Rebecca Han, Nina Tyminksa, Jordan R, Schmidt and David S. Sholl, Journal of Physical Chemistry C, 123 (2019) 6655-6666
77. *Predictions of Hg^0 and $HgCl_2$ 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
78. *Screening diffusion of small molecules in flexible zeolitic imidazolate frameworks using a DFT parameterized force field,* Ross J. Verploegh, Ambarish Kulkarni, Salah Eddine Boulfelfel, Jonathan C. Haydak, Dai Tang and David S. Sholl, Journal of Physical Chemistry C, 123 (2019) 9153-9167
79. *Stability of zeolitic imidazolate frameworks in NO_2,* 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
80. *In silico prediction of structural properties of a racemic porous organic cage crystal,* Yang Liu, Guanghui Zhu, Wenqin You, Hongjian Tang, Christopher W. Jones, Ryan Lively and David S. Sholl, Journal of Physical Chemistry C, 123 (2019) 1720-1729
81. *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
82. *Moving beyond adsorption capacity in design of adsorbents for CO_2 capture from ultradilute feeds: Kinetics of CO_2 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
83. *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
84. *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

85. *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
86. *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
87. **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
88. *First-principles-derived force fields for CH_4 adsorption and diffusion in siliceous zeolites,* Hanjun Fang, Rohan Awati, Salah E. Boulfelfel, Peter I Ravikovitch, and David S. Sholl, Journal of Physical Chemistry C, 122 (2018) 12880-12891
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Books

Non-fiction

Density Functional Theory: A Practical Introduction (2nd ed.), David S. Sholl and Jan Steckel, John Wiley & Sons, 2023 (ISBN: 978-1119840862).
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.
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Success and Creativity in Scientific Research: Amaze Your Friends and Surprise Yourself, David S. Sholl, CRC Press, 2021 (ISBN: 978-0367619183)

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
3. Process for recovering para-xylene using a metal organic framework adsorbent in a simulated moving-bed process, M. Rungta, J. S. Abichandani, D. L. Pilliod, R. G. Tinger, A. Go, K. Zhang, S. Nair, J. Gee, D. Sholl, US Patent 10,358,401, Issued July 23, 2019
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Departmental Seminars and Invited Presentations

1. BTSD/WINGS Career Forum: Long Term Career Vision and Shaping, Oak Ridge National Laboratory, Oak Ridge, TN, May 2023
2. Creating Good Ideas Workshop, Future Leaders and WiNS, Oak Ridge National Laboratory, Oak Ridge, TN, May 2023
3. 3M Tech Forum Climate Chapter, 3M Corporate Research, April 2023 (virtual)
4. University of the Third Age, Armidale, NSW, Australia, April 2023
5. Energy Systems Analysis Graduate Seminar, Department of Mechanical Engineering, University of Maryland, March 2023 (virtual)
6. Kurt Wohl Memorial Lecture, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, February 2023
7. University of Oklahoma Sustainability Forum, University of Oklahoma, Norman, OK, January 2023
8. Oak Ridge Public Library Tech Talk, Oak Ridge, TN, January 2023
9. Chemical Sciences. Geosciences and Biological Sciences seminar, Sandia National Laboratory (virtual), January 2023
10. Encouraging Creative Risk Taking in Your Students, Taylor & Francis Webinar, December 2022
11. Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, December 2022
12. Panel member, Influencing Policy Decisions on Climate Solutions, AIChE Annual Meeting, Phoenix, AZ, November 2022
13. Panel member, Powering The Future, AIChE Annual Meeting, Phoenix, AZ, November 2022
14. Panel member, Regeneration: Healing the Earth to End Climate Change, University of Tennessee Baker Center for Public Policy, Knoxville, TN, November 2022
15. Department of Chemical Engineering Graduate Student Symposium Keynote Talk, Carnegie Mellon University, Pittsburgh, PA, October 2022
16. National Energy Technology Laboratory, Pittsburgh, PA, October 2022
17. Gordon Conference on Chemical Separations, Ventura, CA, October 2022
18. University of Tennessee Science Forum, Knoxville, TN, September 2022
19. Department of Chemical Engineering, University of Queensland, August 2022 (virtual)

20. American Ceramic Society Young Professionals Network, Professional Skills and Personal Development Webinar Series, August 2022 (virtual)
21. Closing the Carbon Cycle Workshop, Pacific Northwest National Laboratory, Richland, WA, July 2022
22. Experience ORNL, Oak Ridge National Laboratory, Oak Ridge, TN, May 2022
23. Texas Tech University CheGSA Distinguished Speaker Series, Dept. of Chemical Engineering, Texas Tech University, April 2022 (virtual)
24. NSF/DOE Workshop on Addressing Rigor and Reproducibility in Heterogeneous Catalysis, April 2022 (virtual)
25. Department of Chemical Engineering, Pennsylvania State University, State College, PA, October 2021
26. Chemical Engineering Alumni Lectures, University of Massachusetts Amherst, September 2021
27. DOE Advanced Manufacturing Office TRANSSFORM Initiative Workshop (virtual meeting), September 2021
28. NRL Workshop on Direct Air Capture and Blue Carbon Removal (virtual meeting), August 2021
29. Symposium on Surface Chemistry and Solvation Effects in Confined Environments, ACS Virtual National Meeting, April 2021
30. Virtual seminar, International Adsorption Society, March 2021
31. Plenary talk, North American Membrane Society 2020 Meeting (virtual meeting), May 2020
32. Department of Chemical and Environmental Engineering, University of Arizona, Tucson, AZ, October 2019
33. Doumas Lecture in Chemical Engineering, Department of Chemical Engineering, Virginia Tech, Blacksburg, VA, October 2019
34. Reproducibility in Science and Engineering, ACS 66th International Symposium, Columbus, OH, October 2019
35. Department of Chemical Engineering, Seoul National University, Seoul, South Korea, October 2019
36. Department of Chemical Engineering, Nanyang University, Singapore, October 2019
37. Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, October 2019
38. Department of Chemical and Biomolecular Engineering, University of Notre Dame, South Bend, IN, September 2019
39. Keynote Lecture, DOE BES Separations PI Meeting, Gaithersburg, MD, September 2019
40. School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ, September 2019
41. School of Chemical & Biomolecular Engineering, Georgia Tech, August 2019
42. Gordon Research Conference on Nanoporous Materials, Andover, NH, August 2019
43. Department of Chemical Engineering, New Mexico State University, Las Cruces, NM, April 2019
44. Department of Chemical Engineering, University of Arkansas, April 2019

45. Symposium on New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations and Theory, ACS National Meeting, Orlando, FL, March 2019
46. George Olah Award Symposium in Honor of Chunshan Song, ACS National Meeting, Orlando, FL, March 2019
47. Department of Chemical Engineering, University of New Hampshire, Durham, NH, March 2019
48. Ma Lecture, Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA, March 2019
49. Physical Sciences Division, Pacific Northwest National Laboratory, Richland, WA, March 2019
50. Department of Chemical Engineering, Oklahoma State University, Stillwater, OK, December 2018
51. University College London, London, UK, December 2018
52. Department of Chemical Engineering, Virginia Commonwealth University, Richmond, VA, October 2018
53. Department of Chemical Engineering, Drexel University, Philadelphia, PA, November 2018
54. Department of Chemical Engineering and Materials Science, University of Alberta, Edmonton, Alberta, October 2018
55. Parr Lecture, Department of Chemical and Biomolecular Engineering, University of Illinois, Champaign, IL, September 2018
56. Plenary Lecture, 15th International Conference on Inorganic Membranes, Dresden, Germany, June 2018
57. Department of Nanoengineering, UCSD, La Jolla, CA, April 2018
58. Department of Chemical Engineering, UC Berkeley, Berkeley, CA, March 2018
59. Department of Chemical Engineering, South Dakota School of Mines, March 2018
60. Plenary Lecture, 2018 US DOE Basic Energy Sciences Separation Science PI Meeting, Gaithersburg, MD, February 2018
61. Material Informatics Seminar, National Institute of Standards, Gaithersburg, MD, February 2018
62. New Vistas in Molecular Thermodynamics, Humboldt Kolleg, Berkeley, CA, January 2018
63. NAS Committee on Reproducibility and Replicability in Science, Washington DC, December 2017
64. Sustainable Engineering Forum Plenary Session, AIChE Annual Meeting, Minneapolis, MN, November 2017
65. Department of Chemical Engineering, MIT, Boston, MA, October 2017
66. Department of Chemical Engineering, Tulane University, New Orleans, LA, September 2017
67. Department of Chemical Engineering, Kansas State University, Manhattan, KS, September 2017
68. Department of Chemical & Petroleum Engineering, University of Kansas, Lawrence, KS, September 2017
69. Sandia National Laboratory, Albuquerque, NM, August 2017

70. ORNL Materials Informatics Workshop, Oak Ridge National Lab, Oak Ridge, TN, August 2017
71. ASEE Summer School for Chemical Engineering Faculty, Raleigh, NC, August 2017
72. Keynote Lecture, Australian CCS Research Conference, Melbourne, VIC, Australia, June 2017
73. AINST Distinguished Seminar, University of Sydney, Sydney, NSW, Australia, June 2017
74. Department of Chemical Engineering, University of New South Wales, Kensington, NSW, Australia, June 2017
75. Department of Physics Colloquium, University of Queensland, Brisbane, QLD, Australia, June 2017
76. CSIRO and University of Monash Department of Chemistry, Clayton, VIC, Australia, May 2017
77. Mieyungah Public Lecture, University of Melbourne, Melbourne, Australia, May 2017
78. Tau Beta Pi Initiates Dinner talk, Georgia Institute of Technology, Atlanta, GA, April 2017
79. Department of Chemical Engineering, University of California Davis, Davis, CA, March 2017
80. Department of Chemical Engineering, Colorado School of Mines, Golden, CO, January 2017
81. Robin H. Stokes Lecture, University of New England, Armidale, NSW, Australia, December 2016
82. Plenary Lecture, Fundamentals and Applications of Advanced Porous Materials Conference, Adelaide, South Australia, Australia, December 2016
83. Department of Chemical and Biological Engineering, University of Delaware, Newark, DE, December 2016
84. Department of Chemical Engineering and Materials Science, Cal Poly Pomona, Pomona, CA, November 2016
85. Department of Chemical Engineering, Texas Tech, Lubbock, TX, November 2016.
86. Georgia Research Alliance Eminent Scholars Annual Meeting, Atlanta, GA, October 2016.
87. Symposium on Supramolecular Assemblies and Metal-Organic Frameworks, SERMACS, Columbia, SC, October 2016.
88. University of Houston Honors College, Houston, TX, October 2016
89. School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, September 2016
90. Department of Chemical Engineering, University College Dublin, Dublin, Ireland, September 2016
91. International Zeolite Membrane Meeting 2016, Dalian, China, August 2016
92. University of Seoul, Seoul, Korea, August 2016
93. Seoul National University, Seoul, Korea, August 2016
94. Board for Chemical Sciences and Technology, National Academy of Sciences, Irvine, CA, August 2016.
95. Gordon Conference on Membranes, New London, NH, August 2016.

96. Gulf Coast and Latin America Scientists Association Seminar Series, Dow Chemical, Freeport, TX, May 2016
97. Savannah River National Laboratory, Aiken, SC, May 2016
98. Symposium on Design, Synthesis and Applications of Advanced Porous Materials, Pacifichem, Honolulu, HI, December 2015
99. Symposium on Data Mining and Machine Learning Meets Experiment and First-principles Simulation for Materials Discovery, Pacifichem, Honolulu, HI, December 2015
100. Symposium on Safety in the Academic Research Laboratory, Pacifichem, Honolulu, HI, December 2015
101. Department of Chemical, Petroleum and Materials Engineering, University of Southern California, Los Angeles, CA, October 2015
102. Department of Chemical and Biomolecular Engineering, University of California Riverside, Riverside, CA, October 2015
103. Department of Chemical and Biomolecular Engineering, University of California Irvine, Irvine, CA, October 2015
104. Department of Chemical Engineering, University of Houston, Houston, TX, October 2015
105. Department of Chemical and Biomolecular Engineering, University of Florida, Gainesville, FL, September 2015
106. Department of Chemical and Biological Engineering, University of Buffalo, Buffalo, NY, September 2015
107. Department of Chemical Engineering, Northeastern University, Boston, MA, August 2015
108. Multiscale Porosity From Laboratory To Industrial Application, 2nd Micromeritics Workshop, Massachusetts Institute of Technology, Cambridge, MA, August 2015
109. School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, August 2015
110. US-Korea Conference on Science, Technology, and Entrepreneurship , Atlanta, GA, July 2015
111. DOE BES Catalysis Contractors Workshop, Annapolis, MD, July 2015
112. Gordon Research Conference on Hydrogen Metal Systems, Stonehill College, MA, July 2015
113. Workshop on Metal-Organic Frameworks, Telluride Scientific Research Conference, Telluride, CO, June 2015.
114. CECAM Workshop on Defects and Disorder in Metal-Organic Frameworks, Chimie ParisTech, Paris, France, June 2015
115. 3M Tech Talk, Minneapolis, MN, May 2015
116. UOP Technical Seminar, Des Plaines, IL, May 2015
117. Department of Chemical Engineering, University of Illinois at Chicago, Chicago, IL, May 2015
118. Symposium on Genomic Approaches to Materials, 249th ACS National Meeting, Denver, CO, March 2015
119. Symposium on Environmental Applications of Metal-Organic Frameworks, 249th ACS National Meeting, Denver, CO, March 2015

120. Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, March 2015
121. Department of Chemical and Biomolecular Engineering, University of South Florida, Tampa, FL, February 2015
122. Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD, December 2014
123. Chinese American Chemical Society Banquet, Atlanta, GA, November 2014
124. Molecular Thermodynamics Plenary Session, AIChE Annual Meeting, Atlanta, GA, November 2014
125. Fossil Fuels Plenary Session, AIChE Annual Meeting, Atlanta, GA, November 2014
126. Department of Chemical and Biomolecular Engineering, Columbia University, New York, NY, November 2014
127. Adsorption Technologies Group, Sasol, Sasolburg, South Africa, November 2014
128. Particle Technology Workshop, University of Cape Town, Cape Town, South Africa, November 2014
129. ExxonMobil Applied Materials Symposium, Hershey, PA, October 2014
130. Department of Chemical and Biomolecular Engineering, University of Colorado, Boulder, CO, October 2014
131. Trotter Distinguished Lecture, Department of Chemical Engineering, University of Tennessee, October 2014
132. Symposium on MOFs for Applications, 248th ACS National Meeting, San Francisco, CA, August 2014
133. School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, August 2014
134. Metal Hydrogen 2014, Manchester, UK, July 2014
135. Department of Chemical Engineering, Imperial College London, London, UK, July 2014
136. Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, July 2014
137. Department of Chemistry, National University of Singapore, Singapore, July 2014
138. Department of Chemical Engineering, University of Melbourne, Melbourne, Australia, June 2014
139. International Conference on Inorganic Membranes (keynote address), Brisbane, Australia, June 2014
140. MRS Spring Meeting, San Francisco, CA, April 2014
141. Florida AVS Meeting, Orlando, FL, March 2014
142. J. H. Hopps 5th Annual Training Symposium, Morehouse College, Atlanta, GA, February 2014
143. Dow Chemical Company, Freeport, TX, January 2014
144. School of Chemistry Colloquium, Georgia Institute of Technology, Atlanta, GA, October 2013
145. Physical Chemistry Seminar, University of Wisconsin, Madison, WI, October 2013
146. Department of Chemical and Biomolecular Engineering, Northwestern University, Evanston, IL, October 2013

147. International Zeolite Membrane Meeting, Jeju Island, South Korea, June 2013
148. Workshop on Adsorption in Compliant Solids, Paris, France, June 2013
149. International Conference on Energy and Sustainability, Hang Zhou, China, May 2013
150. Department of Physics, Oberlin College, Oberlin, OH, May 2013
151. Symposium on CO_2 Capture and Utilization, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013
152. Symposium on Hydrogen Production, Storage, and Utilization, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013
153. Symposium on Identification of Environmental Abiotic and Biotic Reactions Using Computational Chemistry, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013
154. Department of Chemistry, University of Florida, February 2013
155. Georgia Tech Clean Energy Speaker Series, Atlanta, GA, February 2013
156. CSIRO, Clayton, Victoria, Australia, December 2012
157. Dept. of Chemical Engineering, University of Queensland, December 2012
158. Pacific Northwest National Laboratory, December 2012
159. Department of Chemical Engineering, Clemson University, November 2012
160. Physical Chemistry seminar, Department of Chemistry, University College London, London, UK, October 2012
161. Air Capture: Developing Technologies for Carbon Recycling and Negative Emissions, Institution of Mechanical Engineering, London, UK, October 2012
162. MOF2012 Keynote Lecture, Edinburgh, UK, September 2012
163. Foundations of Molecular Modeling and Simulations, Portland, OR, July 2012.
164. NETL ORD Seminar, National Energy Technology Laboratory, Pittsburgh, PA, June 2012.
165. Symposium on Gas Capture Materials, Canadian Society of Chemistry Conference, Calgary, AB, May 2012
166. CNMS Theory Seminar, Oak Ridge National Laboratory, Oak Ridge, TN, May 2012
167. ORNL Reactor Off Gas Group, Oak Ridge National Laboratory, Oak Ridge, TN, May 2012
168. Washington University in St. Louis, Department of Energy, Environment, and Chemical Engineering, April 2012
169. University of South Carolina, Department of Chemical Engineering, Columbia, SC, March 2012
170. Materials Modeling Group, Intel Corporation, Santa Clara, CA, March 2012
171. Symposium on Non-adiabatic Dynamics: Surface Hopping and Beyond (invited talk), 243rd ACS National Meeting, San Diego, CA, March 2012
172. Symposium on High-Throughput Screening Approaches for Catalysts Discovery and Optimization (invited talk), 243rd ACS National Meeting, San Diego, CA, March 2012
173. University of California Berkeley, Carbon Capture Program, February 2012
174. Stanford University, Department of Energy Resources Engineering, February 2012
175. MADE@GT Symposium on Materials Design, Atlanta, GA, November, 2011

176. Georgia Research Alliance Eminent Scholars Annual Meeting, Atlanta, GA, October 2011
177. Department of Chemical Engineering Seminar, University of Kentucky, Louisville, KY, October 2011.
178. Sandia National Laboratory, Microfluidics Department, Livermore, CA, September 2011.
179. Nanoporous Materials VI (plenary presentation), Banff, Canada, August 21-24, 2011.
180. National Summit on Advancing Clean Energy Technologies (invited panelist), Washington DC, May 2011.
181. Workshop on Materials Design in Chemical Compound Space, Institute for Pure and Applied Mathematics, UCLA, Los Angeles, CA, May 2011
182. Symposium on Applications of Metal-Organic Frameworks, MRS Spring Meeting, San Francisco, CA, April 2011
183. APS March Meeting, Dallas, TX, March 2011
184. Department of Chemical Engineering, National University of Singapore, Singapore, February 2011
185. Institute for Atom-efficient Chemical Transformations Workshop, Northwestern University, Evanston, IL, November 2010
186. COMSEF Plenary Session, AIChE Annual Meeting, Salt Lake City, November 2010
187. Open Forum of the Energy and Environment, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, October 2010
188. Neutrons in Catalysis Workshop, Oak Ridge National Laboratory, September 2010
189. Symposium on Nanoporous Materials for Environmental Applications, ACS National Meeting, Boston, August 2010
190. 5th International Zeolite Membrane Meeting, Loutraki, Greece, May 2010.
191. Department of Chemical and Bioengineering, University of Washington, Seattle, WA, May 2010.
192. Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, April 2010.
193. Department of Chemical Engineering, The Pennsylvania State University, State College, PA, April 2010.
194. Keynote Lecture, Symposium on Advances in Membrane Science and Technology, ACS National Meeting, San Francisco, March 2010.
195. Dept. of Chemical Engineering, Texas A&M University, College Station, TX, January 2010.
196. Oak Ridge National Laboratory, Computational Materials Division, Knoxville, TN, January 2010.
197. Thin Films Division, AVS 56th International Symposium, San Jose, November 2009.
198. Dept. of Chemical Engineering, Clemson University, October 2009.
199. DOE Computational Materials Science Network Workshop, Denver, CO, October, 2009.

200. XVIII International Materials Research Congress, Cancun, Mexico, August 2009.
201. US-China Workshop on Surface Science and Heterogeneous Catalysis, Dalian, China, June 2009.
202. Savannah River National Laboratory, Materials Division, Aiken, SC, June 2009.
203. Swedish-American Entrepeneurial Days, Keynote Address, Savannah, GA, April 2009.
204. Emerson Center Annual Symposium, Emory University, March 2009.
205. Dept. of Chemical Engineering, University of Louisville, Louisville, KY, February 2009
206. Center for Simulational Physics, 22nd Annual Workshop, University of Georgia, Athens, GA, February 2009
207. Dept. of Chemical Engineering, University of New South Wales, Sydney , NSW, Australia, December 2008.
208. Dept. of Physics, University of Sydney, Sydney, NSW, Australia, December 2008.
209. Dept of Chemical Engineering, University of Melbourne, Melbourne, Victoria, Australia, December 2008
210. CSIRO Energy Research Center, Brisbane, Queensland, Australia, December 2008
211. Future Directions in Transport, Centennial Symposium, AIChE Annual Meeting, Philadelphia, November 2008.
212. Department of Chemical Engineering, University of Maine, Bangor, ME, October 2008
213. University of Queensland Physics Summer School, Stradbroke Island, Queensland, Australia, December 2008.
214. Center for Nanoscale Materials, Argonne National Laboratory, Chicago, IL, October 2008
215. Center for Simulational Physics, University of Georgia, Athens, GA, October 2008
216. College of Engineering, Peking University, Beijing, China, May 2008.
217. Department of Chemistry, Tsinghua University, Beijing, China, May 2008.
218. Department of Chemical Engineering, Beijing University of Chemical Technology, Beijing, China, May 2008.
219. Department of Chemistry, Emory University, Atlanta, GA, April 2008.
220. Thermodynamics in Chemical Engineering: Prospects and Perspectives, AIChE Spring Meeting, New Orleans, LA, April 2008.
221. Computational Methods and Molecular Modeling in Fuel Chemistry, ACS National Meeting, New Orleans, LA, April 2008.
222. Arthur W. Adamson Award for Distinguished Service of Surface Chemistry: Symposium in Honor of Francisco Zaera, ACS National Meeting, New Orleans, LA, April 2008.
223. Department of Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ, November 2007.
224. Department of Materials Science and Engineering, University of Illinois, Champaign, IL, November 2007.

225. MESD Plenary Session, AIChE Annual Meeting, Salt Lake City, UT, November 2007.
226. CECAM Workshop on Chirality at Surfaces, Lyons, France, October 2007.
227. Symposium on Advanced Materials for Conversion and Separations in Energy Applications, ACS National Meeting, Boston, MA, August 2007.
228. Symposium on Hydrogen Storage and Fuel Cell Technology, ACS National Meeting, Boston, MA, August 2007.
229. Gordon Conference on Hydrogen in Metals, Waterville, Maine, July 10, 2007.
230. Department of Chemical Engineering, Oklahoma University, April 19, 2007
231. Symposium on Capturing Complexity in Physical Sciences Simulation, ACS National Meeting, Chicago, IL, March 27, 2007
232. Symposium on Implications and Applications of Chirality in Physical Chemistry, ACS National Meeting, Chicago, IL, March 28, 2007
233. Department of Chemical Engineering and Materials Science, University of Minnesota, January 23, 2007.
234. Department of Chemistry, Carleton College, January 12, 2007.
235. Biosecurity and Nanosciences Laboratory, Lawrence Livermore National Laboratory, January 10, 2007.
236. COMSEF Plenary Session, AIChE Annual Meeting, San Francisco, California, November 12-16, 2006
237. Department of Chemical Engineering, Carnegie Mellon University, November 2, 2006
238. Department of Chemical Engineering, Vanderbilt University, October 30, 2006.
239. Department of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia, October 18, 2006
240. Metal-Hydrogen 2006, Maui, Hawaii, October 1-6, 2006
241. Symposium on Challenges for the Hydrogen Economy: Storage Science and Technology, ACS National Meeting, San Francisco, California, September 10-14, 2006.
242. Symposium on Chirality and Enantioselectivity at Surfaces, ACS National Meeting, San Francisco, California, September 10-14, 2006.
243. Symposium on Computational Materials Design in Chemical Industries, ACS National Meeting, San Francisco, California, September 10-14, 2006.
244. Gordon Research Conference on Membranes: Materials and Processes, New London, NH, August 6-11, 2006.
245. Gordon Research Conference on Physical Metallurgy, Plymouth, NH, July 23-26, 2006.
246. Gordon Research Conference on Chemistry at Interfaces, Biddeford, Maine, July 9-14, 2006.
247. Department of Physics, University of Sydney, Sydney, NSW, Australia, May 19, 2006.
248. 135th TMS Annual Meeting, March 12-16, 2006, San Antonio, TX.
249. Center for Low Emission Technologies, University of Queensland, Brisbane Australia, December 2005.
250. ARC Center for Functional Nanomaterials 2nd Annual Meeting, Noosa Heads, Australia, December 2005.

251. Department of Chemical Engineering, University of Melbourne, Melbourne, Australia, November 2005.
252. Center for Molecular Modeling, Swinburne University, Melbourne, Australia, November 2005.
253. China/Japan/USA Joint Chemical Engineering Meeting, Beijing, China, October 11-13, 2005.
254. Department of Chemical Engineering, University of Newcastle, Newcastle, Australia, October 2005.
255. CSIRO Energy Center, Newcastle, Australia, October 2005.
256. ExxonMobil Corporate Research, Annandale, NJ, October 2005.
257. Nanoscale Science and Technology Center, Griffith University, Brisbane, Australia, August 2005.
258. Department of Chemical Engineering and Materials Science, Arizona State University, Tempe, AZ, April 2005.
259. Department of Chemical Engineering, City College of New York, New York, NY, February 2005.
260. Department of Materials Science, University of Pittsburgh, Pittsburgh, PA, February 2005.
261. Department of Chemical Engineering, University of Colorado, Boulder, CO, January 2005.
262. Workshop on Molecular and Particle Processes at Solid Surfaces, San Luis, Argentina, November 2004.
263. ExxonMobil Corporate Research, Annandale, NJ, September 2004.
264. 3rd International Zeolite Membrane Meeting, Breckenridge, CO, July 2004.
265. van't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, Holland, May 2004.
266. Surface Science Center, University of Liverpool, Liverpool, UK, May 2004.
267. Department of Chemistry, University of Cardiff, Cardiff, UK, May 2004.
268. Department of Chemistry, University of Sydney, Sydney, NSW, Australia, May 2004.
269. Department of Physics, University of New England, Armidale, NSW, Australia, May 2004.
270. Department of Chemical Engineering, University of Queensland, Brisbane, Qld., Australia, April 2004.
271. Department of Chemical Engineering, Purdue University, West Lafayette, IN, March 2004.
272. Third San Luis Symposium on Surface Science, Merida, Venezuela, March 2004.
273. Department of Chemistry, Wake Forest University, Winston-Salem, NC, February 2004.
274. Department of Chemistry, Duquesne University, Pittsburgh, PA, January 2004.
275. Surface Analysis session, FACSS 2003 Annual Meeting, Ft. Lauderdale, FL, October 2003.
276. Department of Materials Science and Engineering, University of Florida, Gainesville, FL, October 2003.
277. Department of Chemical Engineering, University of Florida, Gainesville, FL, October 2003.

278. Department of Chemical Engineering, University of Buffalo, Buffalo, NY, October 2003.
279. CECAM Workshop on Simulation of Zeolites: Towards In Silico Design, Lyons, France, October 2003.
280. Department of Physics, Indiana University of Pennsylvania, Indiana, PA, September 2003.
281. Chiral Surfaces Symposium, ACS National Meeting, New Orleans, LA, March 2003.
282. Mechanistic Surface Chemistry Symposium, ACS National Meeting, New Orleans, LA, March 2003
283. Department of Chemical Engineering, University of Missouri at Rolla, January 2003.
284. Pittsburgh-Cleveland Catalysis Society, Pittsburgh, PA, December 2002.
285. Department of Chemical Engineering, University of Wisconsin, December 2002.
286. CAST Plenary Session, AIChE Annual Meeting, Indianapolis, IN, November 2002.
287. Department of Chemical Engineering, University of Delaware, October 2002.
288. Pittsburgh AIChE Chapter, October 2002.
289. Materials Research Seminar, Department of Chemical Engineering, The Pennsylvania State University, October 2002.
290. Chemical Physics/Physical Chemistry Seminar, Departments of Chemistry and Physics, University of Maryland, September 2002
291. GE Corporate Research and Development, Albany, NY, September 2002
292. TDA Inc., Wheatridge, CO, June 2002.
293. National Renewable Energy Laboratory, June 2002.
294. Computational Materials and Biology Group, Sandia National Laboratory, Albuquerque, NM, June 2002.
295. Atomic and Molecular Physics Group, T-Division, Los Alamos National Laboratory, May 2002.
296. Department of Chemical Engineering, University of Massachusetts – Amherst, April 2002.
297. Department of Chemical Engineering, University of Akron, February 2002.
298. Air Products R&D Division, January 2002.
299. Department of Chemical Engineering, University of California at Santa Barbara, Santa Barbara, CA, November 2001.
300. Department of Chemistry, Kent State University, Kent, OH, September 2001.
301. Midwest Thermodynamics and Statistical Mechanics Meeting, East Lansing, MI, May 2001.
302. Computational Materials and Biology Group, Sandia National Laboratory, Albuquerque, NM, December 2000.
303. Department of Chemical Engineering, University of Colorado, October 2000.
304. Department of Applied Mathematics, University of Colorado, October 2000.
305. ExxonMobil Corporate Research Division, Annandale, NJ, June 2000.
306. Air Products and Chemicals Technology Division, Allentown, PA, June 2000.
307. Department of Chemical Engineering, University of Tennessee, April 2000.
308. ACS National Meeting, San Francisco, CA, March 2000 (invited presentation).

309. Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA, October 1999.
310. Condensed Matter Seminar, Department of Physics, Carnegie Mellon University, Pittsburgh, PA, October 1998
311. Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, PA, September 1998
312. Department of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, March 1997.
313. Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA, February 1997.
314. Department of Chemistry, Iowa State University, Ames, IA, January 1997.
315. Department of Applied Mathematics, University of Colorado, Boulder, CO, November 1995.
316. Physics Department, University of New England, Armidale, NSW, Australia, December 1993.
317. Department of Physics and Theoretical Physics, Australian National University, Canberra, ACT, Australia, March 1991.

Other Presentations

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 CO_2 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, Rekjavik, 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. 63nd 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 Ultraselective 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 CO_2 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=Bh2bK6zlPdU
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. NASA, "Advanced sorbent system for oxygen recovery from helium", $37,500, 9/1/20-8/31/21 (subcontract from TDA)
2. ExxonMobil Research and Engineering, "Quantitative Predictions of Molecular Transport in Zeolites", $296,000, 10/1/20-10/1/21
3. Sandia National Laboratories, "Smart Materials for Highly Complex Optical Tags with Environmental Response", $187,000, 10/1/19-9/30/22
4. ExxonMobil Research and Engineering, "Computational Modeling of Specific Interactions of Non-hydrocarbon species", $114,000, 11/1/18-11/1/19
5. Department of Energy Basic Energy Sciences, "Combining Molecular Simulations and Machine Learning to Comprehensively Explore Adsorption Space", $528,028, 10/1/19-9/30/22 (Sholl is PI, A. Medford is co-PI) ($264,014 to Sholl group)
6. Department of Energy Advanced Manufacturing Office, "NNMI/RAPID – Focus Area Leader", $200,000, 4/1/17-12/31/20 (subcontract from AIChE)
7. 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)
8. Sandia National Laboratory, "Engineered Materials for Deactivation of Chemical Agents", $118,000, 10/1/17-9/30/19
9. ExxonMobil Research and Engineering, "Quantitative Predictions of Diffusion in Zeolites", $434,000, 4/16/16-4/15/19
10. ExxonMobil Upstream Research, "Modeling Adsorption of Polar Molecules in Complex Adsorbents", $548,000, 10/16/15-10/15/19
11. ExxonMobil Research and Engineering, "Modeling Molecular Transport of Gas and Liquid Mixtures in Microporous Materials", $339,000, 9/6/16-9/14/19
12. 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)
13. 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)
14. 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)
15. 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)
16. 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), 10/1/15-9/30/18 (R. Lively is PI, D. Sholl, K. Walton, Y. Kawajiri, and M. Realff are co-PIs)
17. 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)
18. Oak Ridge National Laboratory, "GO Project: Discovery, Understanding and Validation of Layered Materials", $110,000, 5/1/14-4/30/16

19. Oak Ridge National Laboratory, “GO Project: Layered Ferroics”, $110,000, 9/1/14-8/30/16
20. 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)
21. Department of Energy Energy Frontier Research Center “Center for Understanding and Control of Acid-Gas-Induced Evolution of Materials for Energy (UNCAGE-ME)”, $11,200,000, 8/1/14-7/31/18 (Walton is PI, Sholl is one of 17 co-PIs and Center Deputy Director)
22. 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).
23. ExxonMobil Research and Engineering, “Adsorption in Zeolites”, $820,000, 10/13-10/17
24. Department of Energy Basic Energy Sciences, “Nanoporous Materials Genome Center”, $550,000 (GT share), 11/12-10/17 (L. Gagliardi [U. Minnesota] is PI, Sholl is one of ~10 co-PIs)
25. 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)
26. Phillips66, “Advanced Materials and Membranes for Gas Separations”, $900,000, 10-12-9/15 (Nair is PI, Sholl and Jones are co-PIs)
27. ExxonMobil Chemicals, “Recovery of olefins from naptha using MOFs”, $342,000, 11/12-10/14 (Sholl is PI, Nair is co-PI)
28. ExxonMobil Chemicals, “Identification of MOFs for xylene enrichment”, $378,000, 10/12-9/14 (Sholl is PI, Nair is co-PI)
29. Dow Chemical, “Membrane reactors for hydrocarbon processing”, $2,000,000, 10/10-9/14 (Nair is PI, Jones and Sholl are co-PIs)
30. 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)
31. 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)
32. 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)
33. 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)
34. 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)
35. Sandia National Laboratory, “Computational modeling of nanoporous framework materials”, $240,000, 3/10-8/13
36. 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)

37. 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
38. 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),
39. 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.
40. 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)
41. Dow Corporation, "Ethanol, Propanol and other high alcohol synthesis from H_2/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
42. ConocoPhilips 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
43. 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
44. Department of Energy, Office of Basic Energy Sciences, "Ab initio screening of alloys for hydrogen purification membranes", $450,000, 8/08-7/11.
45. Georgia Tech Creating Energy Options Program, "Amorphous Metal Alloys for Hydrogen Purification Membranes", $38,500, 7/08-6/09
46. National Science Foundation, "The transition state in catalysis: experiment and computational modeling", $494,743, 4/07-2/10 (A. Gellman, PI; Sholl co-PI).
47. 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).
48. 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).
49. 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).
50. Pennsylvania Infrastructure Technology Alliance, "Spectroscopic Characteristics of Nanostructured Chiral Surfaces", $44,000, 9/06-5/08 (A. Gellman, PI; Sholl co-PI).
51. 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.
52. 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).

53. 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).
54. 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).
55. Department of Energy, Basic Energy Sciences, “Rapid ab initio screening of ternary alloys for hydrogen purification”, $300,000, 7/05-6/08.
56. Department of Energy, “First principles quantum chemistry approaches to predicting surface segregation in metal alloy hydrogen membranes”, $50,000, 9/05-8/06.
57. Sandia National Laboratory, “Atomically detailed simulations of molecular mixtures in cationic zeolites”, $20,000, 5/05-9/05.
58. Merck Company Foundation, “Separation of Chiral Compounds Using Chiral Surfaces”, $90,000, 8/04-7/07.
59. 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.
60. 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.
61. 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.
62. Sandia National Laboratory, “Atomically-detailed simulations of mixture adsorption in zeolites”, $30,000, 3/04-9/04.
63. 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).
64. Pennsylvania Infrastructure Technology Alliance, “Computational Thermochemistry of GaAs Contaminants”, $5,500, 11/03-1/04. (Sholl is PI, D. Yaron is co-PI.)
65. ACS Petroleum Research Fund, “Density Functional Theory and Lattice Gas Models of Hydrogen Diffusion in CuPd Alloys”, $80,000, 5/03-8/05.
66. National Science Foundation, "Catalysis and Separations With One Hand", $320,000 (Sholl is PI, A. Gellman is co-PI), 9/02-9/05.
67. 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.
68. ACS Petroleum Research Fund, “Chiral Surfaces Symposium”, $3,600, 3/03-8/03 (on behalf of the ACS Colloids and Surfaces Division).
69. 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.
70. National Science Foundation, “2002 Midwest Thermodynamics and Statistical Mechanics Meeting, May 13-14, 2002, Pittsburgh, PA”, $6400, 5/02-5/03.

71. Camille Dreyfus Teacher-Scholar Award, $60,000, 2002.
72. E. Kears Pollock/PPG Industries Grant for Young Faculty, $100,000, 2002-2005.
73. 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.)
74. 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.
75. Sloan Foundation Fellowship, $40,000, 6/01-5/03.
76. 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).
77. 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.)
78. National Energy Technology Laboratory, Department of Energy, “Computational Screening of Zeolites for CO_2 Sequestration”, $157,402, 3/01-3/03.
79. National Energy Technology Laboratory, Department of Energy, “University/NETL Student Partnership”, $30,000, 9/00-8/01.
80. 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).
81. Air Products and Chemicals Inc., “Fundamental Studies of Molecular Diffusion in Zeolite Cavities”, $15,000, 9/00-8/01.
82. Air Products and Chemicals Inc., “Corrosion of Metal Surfaces by Metal Dusting”, $25,000, 9/00-9/01.
83. National Science Foundation CAREER Award, “Atomically Detailed Modeling of Transport Through Zeolite Membranes”, $215,000, 4/00-3/04
84. American Chemical Society Petroleum Research Fund, “Microscopic Characterization of Adsorption and Transport in Aluminophospate Molecular Sieves”, $20,000, 9/98-8/00.
85. Carnegie Mellon Faculty Development Fund, “Rational Design of Microporous Membranes using Zeolites and Pore-forming Proteins”, $5,814, 4/98-4/99.
86. National Science Foundation, "Catalysis With One Hand", $315,000 (Sholl is PI, A. Gellman is co-PI), 6/99-5/02.
87. National Science Foundation, “Morphological Instability in CdTe Homoepitaxy”, $100,000 (P. Sides is PI, Sholl is co-PI), 7/99-6/00.
88. Carnegie Mellon Interdisciplinary Course Development Fund, "Development of an Interdisciplinary Course on Molecular Simulations, $7,500, 7/99-5/00.

Professional Activities

Journal editing:

- Editor-in-Chief, *AIChE Journal*, 2021-present
- Senior editor, *Langmuir*, 2009-2019 (~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 (2014-1019)
- 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
Organizing Committee, Chemical Engineering National Diversity Equity Workshop, 2021
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
Panel member, National Academies Study Committee, Chemical Engineering: Challenges and Opportunities in the 21sy Century, 2020-2021
Panel lead, DOE BES Basic Research Needs Workshop on Advanced Manufacturing, February 2020
Panel member, National Academies Study Committee, Research Agenda for a New Era in Separations Science, 2018-2019
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 CO_2 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 Kassaee [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 (GradDavid uated 5/2019) [McKinsey]
42. Mayank Agrawal (Graduated 12/2019) [Brown University]
43. Jongwoo Park (Graduated 12/2019) [NETL]
44. Omar Knio (Graduated 5/2020) [3M]
45. John Findley (Graduated 8/2020) [Georgia Tech]
46. Wenqin You (Graduated 5/2020) [Dow]
47. Yuhan Yang (Graduated 8/2022)
48. Ifayoyinsola (Yoyin) Ibikunle (Graduated 5/2023)
49. Zhenzi Yu (expected graduation: 8/2023)
50. Alan Daou (expected graduation: 5/2024)
51. Arvind Ganesan [co-advised with Sankar Nair] (expected graduation: 8/2023)
52. Xuqing Cai (expected graduation: 12/2023)
53. Chao-Wen Chang (expected graduation: 5/2024)
54. Shubham Jamdade (expected graduation: 5/2024)

55. Xiaohan Yu (expected graduation: 5/2024)
56. Akriti Sarswat [co-advised with Ryan Lively] (expected graduation: 5/2025)
57. Jia Yuan Chng (expected graduation: 5/2025)
58. Logan Brabson (expected graduation: 5/2025) [co-advised with AJ Medford]

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)

Undergraduate Students Supervised [Postgraduate placement if known]
Stewart Fronk (1/19-12/19)
Vikram Gopal (1/17-12/17)
Adithya Krishnachand (1/17-12/17)
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, 1/16-3/22
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, 6/18-11/22
24. Dr. Raghuram Thyagarajan, 8/18-
25. Dr. Jifeng Sun, 11/18-