Curriculum Vitae – David S. Sholl

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Contact information
Oak Ridge National Laboratory, Oak Ridge, TN 37831
Email: shollds@ornl.gov
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology
Atlanta, GA 30332-0100, USA
Email: david.sholl@chbe.gatech.edu

Georgia Tech research group information: sholl.chbe.gatech.edu

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

Awards and Distinctions

1. Chemical Engineering Alumni Lectures, University of Massachusetts Amherst (2021)
2. Fellow, American Association for the Advancement of Science (2020)
3. Doumas Lecture in Chemical Engineering, Virginia Tech (2019)
4. Fellow, American Institute of Chemical Engineering (2019)
5. Institute Award for Excellence in Industrial Gases Technology, American Institute of Chemical Engineering (2018)
6. Parr Lecturer, Department of Chemical and Biomolecular Engineering, University of Illinois (2018)
7. "Highly Prolific Author" recognition, Journal of Physical Chemistry C (2017)
8. AIChE Gary Leach Award [jointly with several faculty and staff from Georgia Tech] (2015)
9. Early Career Achievement Award, Computational Molecular Science and Engineering Forum, AIChE (2010)
10. DOE Hydrogen Program R&D Award (2008)
11. MESD Plenary Session speaker, AIChE Annual Meeting (2007)

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

Research Publications (> 21,400 citations, h-index = 79 as reported by Web of Science)
[Publications with > 50 citations indicated by * and with > 100 citations indicated by **]

1. *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
2. *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
3. *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
4. *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
5. *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
6. *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
7. *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

8. *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
9. *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
10. *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
11. *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
12. *A database of porous rigid amorphous materials,* Raghuram Thyagarajan and David S. Sholl, Chemistry of Materials, 32 (2020) 8020-8033
13. *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
14. *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
15. *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
16. *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
17. *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
18. *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
19. *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
20. *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

21. *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
22. *Watching Water, Sodium, and Chloride Passing through a Graphitic Pore,* David S. Sholl, Matter, 2 (2020) 524-525
23. *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
24. *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
25. *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
26. *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
27. *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
28. *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
29. *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
30. *Five easy ways to make your research more reproducible,* David S. Sholl, Langmuir, 35 (2019) 13257-13258
31. *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
32. *In-situ ATR-IR study of surface reaction during aqueous phase reforming of glycerol, sorbitol and glucose over Pt/γ-Al_2O_3,* Molecular Catalysis, 475 (2019) 110423
33. *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
34. *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

35. *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
36. *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
37. *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
38. *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
39. *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
40. *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
41. *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
42. *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
43. *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
44. *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
45. *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
46. *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

47. *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
48. *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
49. *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
50. *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
51. *The effect of aluminum short-range ordering on carbon dioxide adsorption in zeolites,* John M. Findley, Peter I. Ravikovitch and David S. Sholl, Journal of Physical Chemistry C, 122 (2018) 12332-12340
52. *Efficiently exploring adsorption space to identify privileged adsorbents for chemical separations of a diverse set of molecules,* Dai Tang, Ying Wu, Ross J. Verploegh and David S. Sholl, ChemSusChem, 11 (2018) 1567-1575
53. *Competitive binding of ethylene, water, and carbon monoxide in metal-organic framework materials with open Cu sites,* Wenqin You, Yang Liu, Joshua D. Howe and David S. Sholl, Journal of Physical Chemistry C, 122 (2018) 8960-8966
54. *Quantitative predictions of molecular diffusion in binary mixed-linker zeolitic imidazolate frameworks using molecular simulation,* Ross J. Verploegh, Ying Wu, Salah Eddine Boulfelfel and David S. Sholl, Journal of Physical Chemistry C, 122 (2018) 5627-5638
55. *Insights into the stability of zeolitic imidazolate frameworks in humid acidic environments from first-principles calculations,* Chu Han, Chenyang Zhang, Nina Tyminska, J. R. Schmidt and David S. Sholl, Journal of Physical Chemistry C, 122 (2018) 4339-4348
56. *Writing theory and modeling papers for Langmuir: The good, the bad and the ugly (Editorial),* Han Zuilhof, Shu-Hong Yu and David S. Sholl, Langmuir 34 (2018) 1817-1818
57. *Liquid-phase multicomponent adsorption and separation of xylene mixtures by flexible MIL-53 adsorbents,* Mayank Agrawal, Souryadeep Bhattacharyya, Yi Huang, Krishna C. Jayachandrababu, Christopher R. Murdock, Jason A. Bentley, Alejandra Rivas-Cardona, Machteld M. Mertens, Krista S. Walton, David S. Sholl and Sankar Nair, Journal of Physical Chemistry C, 122 (2018) 386-397
58. *Formation mechanisms and defect engineering of imine-based porous organic cages,* Guanghui Zhu, Yang Liu, Luis Flores, Zachary R. Lee, Christopher W. Jones, David A. Dixon, David S. Sholl and Ryan P. Lively, Chemistry of Materials, 30 (2018) 262-272
59. **How reproducible are isotherm measurements in metal-organic frameworks?* Jongwoo Park, Joshua D. Howe and David S. Sholl, Chemistry of Materials, 29 (2017) 10487-10495

60. *CO_2 dynamics in pure and mixed-metal MOFs with open metal sites,* Robert M. Marti, Joshua D. Howe, Cody R. Morelock, Mark S. Conradi, Krista S. Walton, David S. Sholl and Sophia E. Hayes, Journal of Physical Chemistry C, 121 (2017) 25778-25787
61. *Research challenges in avoiding "showstoppers" in developing materials for large-scale energy applications,* Krista S. Walton and David S. Sholl, Joule, 1 (2017) 208-211
62. *Heat-treatment of defective UiO-66 from modulated synthesis: Adsorption and stability studies,* Yang Jiao, Yang Liu, Guanghui Zhu, Julian T. Hungerford, Souryadeep Bhattacharyya, Ryan P. Lively, David S. Sholl and Krista S. Walton, Journal of Physical Chemistry C, 121 (2017) 23471-23479
63. *Recovery of acid-gas-degraded zeolitic imidazolate frameworks by solvent-assisted crystal redemption (SACRed),* Krishna C. Jayachandrababu, Souryadeep Bhattacharyya, Yadong Chiang, David S. Sholl and Sankar Nair, ACS Applied Materials and Interfaces, 9 (2017) 34597-34602
64. *Computational screening of functionalized UiO-66 materials for selective contaminant removal from air,* Hakan Demir, Krista S. Walton and David S. Sholl, Journal of Physical Chemistry C, 121 (2017) 20396-20406
65. *Effect of surface structure of TiO_2 nanoparticles on CO_2 adsorption and SO_2 resistance,* Uma Tumuluri, Joshua D. Howe, William P. Mounfield, Meijun Li, Miaofang Chi, Zachary D. Hood, Krista S. Walton, David S. Sholl, Sheng Dai and Zili Wu, ACS Sustainable Chemistry & Engineering, 5 (2017) 9295-9306
66. *Butanol separation from humid CO_2-containing multicomponent vapor mixtures by zeolitic imidazolate frameworks,* Souryadeep Bhattacharyya, Krishna C. Jayachandrababu, Yadong Chiang, David S. Sholl and Sankar Nair, ACS Sustainable Chemistry & Engineering, 5 (2017) 9467-9476
67. *Modeling and process simulation of hollow fiber membrane reactor systems for propane dehydrogenation,* Seung-Won Choi, David S. Sholl, Sankar Nair, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, John G. Prendergast, AIChE Journal 63 (2017) 4519-4531
68. *Hierarchical Ga-MFI catalysts for propane dehydrogenation,* Wun-gwi Kim, Jungseob So, Seung-Won Choi, Yujun Liu, Ravindra S. Dixit, Carsten Sievers, David S. Sholl, Sankar Nair and Christopher W. Jones, Chemistry of Materials, 29 (2017) 7213-7322
69. *Towards the directional transport of molecules on surfaces,* Natalie A. Wasio, Colin J. Murphy, Dipna A. Patel, Daniel Wei, David S. Sholl and E. Charles H. Sykes, Tetrahedron, 73 (2017) 4858-4863
70. *Impacts of gas impurities from pipeline natural gas on methane storage in metal-organic frameworks during long-term cycling,* Ying Wu, Dai Tang, Ross J. Verploegh, Hongxia Xi and David S. Sholl, Journal of Physical Chemistry C, 121 (2017) 15735-15745
71. *Lattice-gas modeling of adsorbate diffusion in mixed-linker zeolitic imidazolate frameworks: Effect of local imidazolate ordering,* Ross J. Verploegh, Ying Wu and David S. Sholl, Langmuir, 33 (2017) 6481-6491

72. *First-principles investigation of chemical stability and proton conductivity in M-doped $BaZrO_3$ (M = K, Rb, and Cs),* Journal of the American Ceramic Society, 100 (2017) 2997-3003
73. *Establishing upper bounds on CO_2 swing capacity in sub-ambient pressure swing adsorption via molecular simulation of metal-organic frameworks,* Jongwoo Park, Ryan P. Lively and David S. Sholl, Journal of Materials Chemistry A, 5 (2017) 12258-12265
74. *Temperature-regulated guest admission and release in microporous materials,* Gang Li, Jin Shang, Qinfen Gu, Rohan V. Awati, Nathan Jensen, Andrew Grant, Xueying Zhang, David S. Sholl, Jefferson Z. Liu, Paul A. Webley and Eric F. May, Nature Communications, 8 (2017) 15777
75. *Monolith-supported amine-functionalized Mg_2(dobpdc) adsorbents for CO_2 capture,* Lalit A. Darunte, Yuri Terada, Christopher R. Murdock, Krista S. Walton, David S. Sholl, and Christopher W. Jones, ACS Applied Materials and Interfaces, 9 (2017) 17043-17051
76. **Structural and mechanistic differences in mixed-linker zeolitic imidazolate framework synthesis by solvent assisted linker exchange and de novo routes,* Krishna C. Jayachandrababu, David S. Sholl and Sankar Nair, Journal of the American Chemical Society, 139 (2017) 5906-5915
77. *Acid gas adsorption on metal-organic framework nanosheets as a model of an "all-surface" material,* Joshua D. Howe, Yang Liu, Luis Flores, David A. Dixon and David S. Sholl, Journal of Chemical Theory and Computation, 13 (2017) 1341-1350
78. ***From water to organics in membrane separations,* Ryan P. Lively and David S. Sholl, Nature Materials 16 (2017) 276-279
79. *Understanding structure, metal distribution, and water adsorption in mixed-metal MOF-74,* Joshua D. Howe, Cody R. Morelock, Yang Jiao, Karena W. Chapman, Krista S. Walton and David S. Sholl, Journal of Physical Chemistry C, 121 (2017) 627-635
80. **Large-scale refinement of metal organic framework structures using DFT,* Chemistry of Materials, Dalar Nazarian, Jeffrey S. Camp, Yongchul G. Chung, Randall Q. Snurr and David S. Sholl, Chemistry of Materials, 29 (2017) 2521-2528
81. *Computational investigation on CO_2 adsorption in titanium carbide-derived carbons with residual titanium,* Difan Zhang, Michael R. Dutzer, Tao Liang, Alexandre F. Fonseca, Ying Wu, Krista S. Walton, David S. Sholl, Amir H. Farmahini, Suresh K. Sinnott, and Susan B. Sinnott, Carbon, 111 (2017) 741-751
82. *Characterizing chemical stability and proton conductivity of B-site doped barium hafnate ($BaHfO_3$) and barium stannate ($BaSnO_3$) with first principles modeling,* Sung Gu Kang and David S. Sholl, Journal of Alloys and Compounds, 693 (2017) 738-743
83. **Propane dehydrogenation catalyzed by gallosilicate MFI zeolites with perturbed acidity,* Seung-Won Choi, Wun-Gwi Kim Jung-Seob So, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, John G. Pendergast, Carsten Sievers, David S. Sholl, Sankar Nair, and Christopher W. Jones, Journal of Catalysis, 345 (2017) 113-123
84. *Computational model and characterization of stacking faults in ZIF-8 polymorphs,* Rebecca Han and David S. Sholl, Journal of Physical Chemistry C, 120 (2016) 27380-27388

85. **Interactions of SO_2-containing acid gases with ZIF-8: Structural changes and mechanistic investigations,* Souryadeep Bhattacharyya, Simon H. Pang, Michael R. Dutzer, Ryan P. Lively, Krista S. Walton, David S. Sholl and Sankar Nair, Journal of Physical Chemistry C, 120 (2016) 27221-27229
86. *Synergistic effects of water and SO_2 on degradation of MIL-125 in the presence of acid gases,* William P. Mounfield III, Chu Han, Simon H. Pang, Uma Tumuluri, Yang Jiao, Souryadeep Bhattacharyya, Michael R. Dutzer, Sankar Nair, Zili Wu, David S. Sholl and Krista S. Walton, Journal of Physical Chemistry C, 120 (2016) 27230-27240
87. *Screening of copper open metal site MOFs for olefin/paraffin separations using DFT-derived force fields,* Ambarish Kulkarni and David S. Sholl, Journal of Physical Chemistry C, 120 (2016) 23044-23054
88. **Facet-specific stability of ZIF-8 in the presence of acid gases dissolved in aqueous solution,* Simon H. Pang, Chu Han, David S. Sholl, Christopher W. Jones, and Ryan P. Lively, Chemistry of Materials, 28 (2016) 6960-6967
89. *One-Step Synthesis of Zeolite Membranes Containing Catalytic Metal Clusters,* Seok-Jhin Kim, Shuai Tan, Micaela Taborga Claure, Laura Gil Briones, Karren L. More, Yujun Liu, Jason S. Moore, Ravindra S. Dixit, John G. Pendergast, David S. Sholl, Christopher W. Jones and Sankar Nair, ACS Applied Materials and Interfaces, 37 (2016) 24671-24681
90. **Propane dehydrogenation over alumina-supported iron/phophorous catalysts: Structural evolution of iron species leading to high activity and propylene selectivity,* Shuai Tan, Bo Hu, Wun-Gwi Kim, Simon H. Pang, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, John G. Pendergast, David S. Sholl, Sankar Nair, Christopher W. Jones, ACS Catalysis, 6 (2016) 5673-5683
91. *Engineering porous organic cage crystals with increased acid gas resistance,* Guanghui Zhu, Christopher D. Hoffman, Yang Liu, Souryadeep Bhattacharyya, Uma Tumuluri, Melinda L. Jue, Zili Wu, David S. Sholl, Sankar Nair, Christopher W. Jones, Ryan P. Lively, Chemistry European Journal, 22 (2016) 10743-10747
92. *Improved Hill-Sauer force field for accurate description of pores in 8-ring zeolites,* Salah Eddine Boulfelfel, Peter I. Ravikovitch, Lucas Koziol, and David S. Sholl, Journal of Physical Chemistry C, 120 (2016) 14140-14148
93. **Direct air capture of CO_2 using amine-functionalized sorbents,* Lalit A. Darunte, Krista S. Walton, David S. Sholl and Christopher W. Jones, Current Opinion in Chemical Engineering, 12 (2016) 82-90
94. *Structure elucidation of mixed-linker zeolitic imidazolate frameworks by solid-state H^1 CRAMPS NMR spectroscopy and modeling,* Krishna C. Jayachandrababu, Ross J. Verploegh, J. Leisen, Ryan C. Nieuwendaal, David S. Sholl and Sankar Nair, Journal of the American Chemical Society, 138 (2016) 7325-7336
95. *Thin hydrogen-selective SAPO-34 zeolite membranes for enhanced conversion and selectivity in propane dehydrogenation membrane reactors,* Seok-Jhin Kim, Yujun Liu, Jason S. Moore, Ravindra S. Dixit, John G. Pendergast, David S. Sholl, Christopher W. Jones, Sankar Nair, Chemistry of Materials, 28 (2016) 4387-4402
96. *Identification of high-CO_2-capacity cationic zeolites by accurate computational screening,* Hanjun Fang, Ambarish Kulkarni, Preeti Kamakoti, Rohan Awati, Peter I. Ravikovitch, and David S. Sholl, Chemistry of Materials, 28 (2016) 3887-3896

97. *Computational identification and experimental evaluation of metal-organic frameworks for xylene enrichment,* Jason A. Gee, Ke Zhang, Souryadeep Bhattacharyya, Jason Bentley, Meha Rungta, Jeevan S. Abichandani, David S. Sholl and Sankar Nair, Journal of Physical Chemistry C, 120 (2016) 12075-12082
98. **Direct air capture of CO_2 using amine functionalized MIL-101(Cr),* Lalit A. Darunte, Aloysius D. Oetomo, Krista S. Walton, David S. Sholl and Christopher W. Jones, ACS Sustainable Chemistry & Engineering, 4 (2016) 5761-5768
99. *Effects of Open Metal Site Availability on Adsorption Capacity and Olefin/Paraffin Selectivity in the Metal-Organic Framework $Cu_3(BTC)_2$,* Jason Bentley, Guo Shiou Foo, Meha Rungta, Sangar Neeraj, Carsten Sievers, David S. Sholl, and Sankar Nair, Industrial and Engineering Chemistry Research, 55 (2016) 5043-5053
100. ***Seven Chemical Separations To Change The World,* David S. Sholl and Ryan P. Lively, Nature, 532 (2016), 435-437
101. **A Comprehensive Set of High-Quality Point Charges for Simulations of Metal-Organic Frameworks,* Dalar Nazarian, Jeffrey S. Camp, and David S. Sholl, Chemistry of Materials, 28 (2016) 785-793
102. *Transition State Theory methods to measure diffusion in flexible nanoporous materials: Application to a porous organic cage crystal,* Jeffrey Camp and David S. Sholl, Journal of Physical Chemistry C, 120 (2016) 1110-1120
103. *Effect of framework flexibility on C_8 aromatic adsorption at high loadings in metal-organic frameworks,* Jason A. Gee and David S. Sholl, Journal of Physical Chemistry C, 120 (2016) 370-376
104. **Computational characterization of defects in metal-organic frameworks: Spontaneous and water-induced point defects in ZIF-8,* Chenyang Zhang, Chu Han, David S. Sholl, and J. R. Schmidt, Journal of Physical Chemistry Letters, 7, (2016) 459-464
105. *Temperature and loading-dependent diffusion of light hydrocarbons in ZIF-8 as predicted through fully flexible molecular simulations,* Ross Verploegh, Sankar Nair and David S. Sholl, Journal of the American Chemical Society, 137 (2015) 15760-15771
106. *Propane dehydrogenation over In_2O_3-Ga_2O_3-Al_2O_3 Mixed Oxides,* Shuai Tan, Seok-Jhin Kim, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, John G. Prendegast, David S. Sholl, Sankar Nair, and Christopher W. Jones, ChemCatChem, 8 (2016) 214-221
107. *High T_c layered ferrielectric crystals by coherent spinodal decomposition,* Michael A. Susner, Alex Belianinov, Albina Borisevich, Qian He, Marius Chyasnavichyus, Hakan Demir, David S. Sholl, Panchapakesan Ganesh, Douglas L. Abernathy, Michael A. McGuire and Petro Maksymovch, ACS Nano, 9 (2015) 12365-12373
108. *Large-scale computational screening of binary intermetallics for membrane-based hydrogen separation,* Nita Chandrasekhar and David S. Sholl, Journal of Physical Chemistry C, 119 (2015) 26319-26326
109. *DFT-based force field development for noble gas adsorption in metal organic frameworks,* Hakan Demir, Jeffrey A. Greathouse, Chad L. Steiger, John J. Perry IV, Mark D. Allendorf and David S. Sholl, Journal of Materials Chemistry A, 3 (2015) 23539-23548

110. *Benchmarking density functional theory predictions of framework structures and properties in a chemically diverse test set of metal-organic frameworks,* Dalar Nazarian, P. Ganesh and David S. Sholl, Journal of Materials Chemistry A, 3 (2015) 22432-22440
111. **Defects in metal-organic frameworks: Challenge or opportunity?,* David S. Sholl and Ryan P. Lively, Journal of Physical Chemistry Letters, 6 (2015) 3437-3444
112. *Computational identification of descriptors for selectivity in syngas reactions on a Mo_2C catalyst,* Liwei Li and David S. Sholl, ACS Catalysis, 5 (2015) 5174-5185
113. ***Predicting multicomponent adsorption: 50 years of the ideal adsorbed solution theory,* Krista S. Walton and David S. Sholl, AIChE Journal, 61 (2015) 2757-2762
114. *DFT-derived force fields for modeling hydrocarbon adsorption in MIL-47(V),* Ambarish R. Kulkarni and David S. Sholl, Langmuir, 31 (2015) 8453-8468
115. *Efficient calculation of gas diffusivity in single-component and binary mixtures of spherical adsorbates in flexible 8MR zeolites,* Rohan V. Awati, Peter I. Ravikovitch, and David S. Sholl, Journal of Physical Chemistry C, 119 (2015) 16596-16605
116. *Prediction of adsorption properties of cyclic hydrocarbons in MOFs using DFT-derived force fields,* Jason A. Gee and David S. Sholl, Journal of Physical Chemistry C, 119 (2015) 16920-16926
117. *Modeling diffusion of linear hydrocarbons in silica zeolite LTA using transition path sampling,* Salah Eddine Boulfelfel, Peter I. Ravikovitch, and David S. Sholl, Journal of Physical Chemistry C, 119 (2015) 15643-15653
118. *Catalytic propane dehydrogenation of In_2O_3-Ga_2O_3 mixed oxides,* Shuai Tan, Laura Briones Gil, Nachal Subramanian, David S. Sholl, Sankar Nair, Christopher W. Jones, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, John G. Prendegast, Applied Catalysis A, 498 (2015) 167-175
119. *Fluorinated carbide-derived carbon: More hydrophilic, yet apparently more hydrophobic,* Amir H. Farmahini, David S. Sholl, and Suresh K. Bhatia, Journal of the American Chemical Society, 137 (2015) 5969-5979
120. *Computational prediction of metal organic frameworks suitable for molecular infiltration as a route to development of conductive materials,* Xiaowa Nie, Ambarish Kulkarni, and David S. Sholl, Journal of Physical Chemistry Letters, 6 (2015) 1586-1591
121. *Molecular design of amorphous porous organic cages for enhanced gas storage,* J. D. Evans, D. M. Huang, M. R. Hill, C. J. Sumby, D. S. Sholl, A. W. Thornton, and C. J. Doonan, J. Phys. Chem. C 119 (2015) 7746-7754
122. *Selection of surface coatings for high H_2 permeability group 5 metal membranes using first-principles calculations,* Rongshun Zhu, Shiqiang Hao, and David S. Sholl, J. Phys. Chem. C 119 (2015) 7848-7855
123. ***Highly tunable molecular sieving and adsorption properties of mixed-linker zeolitic imidazolate frameworks,* Kiwon Eum, Krishna C. Jayachandrababu, Fereshteh Rashidi, Ke Zhang, Johannes Leisen, Samuel Graham, Ryan P. Lively, Ronald R. Chance, David S. Sholl, Christopher W. Jones and Sankar Nair, Journal of the American Chemical Society, 137 (2015) 4191-4197
124. *Impact of branching on the supramolecular assembly of thioethers on Au(111),* Colin J. Murphy, Xuerong Shi, April D. Jewell, Allister F. McGuire, Darin O.

Bellisario, Ashleigh E. Baber, Heather L. Tierney, Emily A. Lewis, David S. Sholl, and E. Charles H. Sykes, Journal of Chemical Physics, 142 (2015) 101915

125. *Material properties and operating configurations of membrane reactors for propane dehydrogenation,* Seung-Won Choi, Christopher W. Jones, Sankar Nair, David S. Sholl, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, and John G. Prendegast, AIChE Journal, 61 (2015) 922-935
126. ***The materials genome in action: identifying the performance limits for methane storage,* Cory M. Simon, Jihan Kim, Diego A. Gomez-Gualdron, Jeffrey S. Camp, Yongchul G. Chung, Richard L. Martin, Rocio Mercado, Michael W. Deem, Dan Gunter, Maciej Haranczyk, David S. Sholl, Randall Q. Snurr, and Berend Smit, Energy & Environmental Science 8 (2015) 1190-1199
127. *First-principles screening of complex transition metal hydrides for high temperature applications,* Kelly M. Nicholson and David S. Sholl, Inorganic Chemistry, 53 (2014) 11833-11848
128. *First-principles prediction of new complex transition metal hydrides for high temperature applications,* Kelly M. Nicholson and David S. Sholl, Inorganic Chemistry, 53 (2014) 11849-11860
129. **Computation-ready, Experimental Metal-Organic Frameworks: A tool to enable high-throughput screening of nanoporous crystals,* Yongchul G. Chung, Jeffrey Camp, Maciej Haranczyk, Benjamin J. Sikora, Wojciech Bury, Vaiva Krungleviciute, Taner Yildirim, Omar K. Farha, David S. Sholl, and Randall Q. Snurr, Chemistry of Materials, 26 (2014) 6185-6192
130. *Powered by DFT: Screening methods that accelerate materials development for hydrogen in metals applications,* Kelly M. Nicholson, Nita Chandrasekhar, and David S. Sholl, Accounts of Chemical Research, 47 (2014) 3275-3283
131. *Control of metal organic framework crystal topology by ligand functionalization: Functionalized HKUST-1 derivatives,* Yang Cai, Ambarish R. Kulkarni, You-Gui Huang, David S. Sholl, and Krista S. Walton, Crystal Growth and Design, 14 (2014) 6122-6128
132. *Contributions of dispersion forces to R-3-methylcyclohexanone physisorption on low and high Miller index Cu surfaces,* D. S. Wei, B. S. Mhatre, A. J. Gellman, and D. S. Sholl, Surface Science, 629 (2014) 35-40
133. *Computational study of hydrogen induced lattice rearrangement and its influence on hydrogen permeance in Pd-Au alloys,* Nita Chandrasekhar and David S. Sholl, J. Alloys Compounds, 609 (2014) 244-252
134. *First principles prediction of ternary interstitial hydride phase stability in the Th-Zr-H system,* K. M. Nicholson and D. S. Sholl, J. Chem. Eng. Data, 59 (2014) 3232-3241
135. *Investigating energetics of Au_8 on graphene/Ru(0001) using a genetic algorithm and density functional theory,* D. Teng, L. B. Vilhelmsen, and D. S. Sholl, Surface Science, 628 (2014) 98-103
136. *Synthesis, characterization, and computation of catalysts at the Center for Atomic-Level Catalyst Design,* J. J. Spivey, K. S. Krishna, C. S. S. R. Kumar, K. M. Dooley, J. C. Flake, L. H. Haber, Y. Xu, M. J. Janik, S. B. Sinnott, Y.-T Cheng, T. Liang, D. S. Sholl, T. A. Manz, U. Diebold, G. S. Parkinson, D. A. Bruce, and P. de Jongh, J. Phys. Chem. C, 118 (2014) 20043-20069

137. **Crystal-size-dependent structural transitions in nanoporous crystals: Adsorption-induced transitions in ZIF-8,* C. Zhang, J. A. Gee, D. S. Sholl, and R. P. Lively, J. Phys. Chem. C, 118 (2014) 20727-20733
138. ***Role of Lewis and Bronsted acid sites in the dehydration of glycerol over niobia,* G. S. Foo, D. Wei, D. S. Sholl, and C. Sievers, ACS Catalysis, 4 (2014) 3180-3192
139. *First-principles study of chemical stability of the lithium oxide garnets $Li_7La_3M_2O_{12}$ (M = Zr, Sn, or Hf),* S. G. Kang and D. S. Sholl, J. Phys. Chem. C, 118 (2014) 17402-17406
140. **Molecular dynamics simulation of framework flexibility effects on noble gas diffusion in HKUST-1 and ZIF-8,* M. V. Parkes, H. Demir, S. L. Teich-McGoldrick, D. S. Sholl, J. A. Greathouse, and M. D. Allendorf, Microporous and Mesoporous Materials, 194 (2014) 190-199
141. *Adsorption and diffusion of Rh and Au dimers and trimers on graphene/Ru(0001),* Dieh Teng and David S. Sholl, Surface Science, 626 (2014) 6-13
142. *Equilibrium adsorption of D- and L-Alanine mixtures on naturally chiral $Cu\{3,1,17\}^{(R\&S)}$ surfaces,* Y. J. Yun, D. Wei, D. S. Sholl, and A. J. Gellman, J, Phys. Chem. C, 118 (2014) 14597-14966
143. *First principles studies of proton conduction in $KTaO_3$,* Sung Gu Kang and David S. Sholl, J. Chem. Phys., 141 (2014) 024707
144. **Thermal, oxidative and CO_2 induced degradation of primary amines used for CO_2 capture: Effect of alkyl linker on stability,* S. A. Didas, R. Zhu, N. A. Brunelli, D. S. Sholl, and C. W. Jones, J. Phys. Chem. C, 118 (2014) 12302-12311
145. *Investigation of the adsorption of amino acids on Pd(111): A density functional theory study,* J. N. James, J. W. Han, and D. S. Sholl, Applied Surface Science, 301 (2014) 199-207
146. *Quantitative computational screening of Pd-based intermetallic membranes for hydrogen separation,* Nita Chandrasekhar and David S. Sholl, J. Membrane Science, 453 (2014) 516-524
147. *Adsorption and diffusion of 4d and 5d transition metal adatoms on graphene/Ru(0001) and the implications for cluster nucleation,* B. F. Habernicht, D. Teng, L. Semidey-Flecha, and D. S. Sholl, Topics in Catalysis 57 (2014) 69-69
148. **Recent developments in first-principles force fields for molecules in nanoporous materials,* Hanjun Fang, Hakan Demir, Preeti Kamakoti, and David S. Sholl, J. Materials Chemistry A, 2 (2014) 274-291
149. *First principles methods for elpasolite halide crystal structure prediction at finite temperatures,* Kelly M. Nicholson, Sung Gu Kang, and David S. Sholl, J. Alloys and Compounds, 577 (2013) 463-468
150. *Predicting low pressure O_2 adsorption in nanoporous framework materials for sensing applications,* Todd R. Zeitler, Timothy van Heest, David S. Sholl, Mark D. Allendorf, and Jeffery A. Greathouse, ChemPhysChem 14 (2013) 3740-3750
151. ***Exploring the framework hydrophobicity and flexibility of ZIF-8: From biofuel recovery to hydrocarbon separations,* Ke Zhang, Ryan P. Lively, Chen Zhang, Ronald R. Chance, William J. Koros, David S. Sholl, and Sankar Nair, Journal of Physical Chemistry Letters, 4 (2013) 3618-3622

152. *Long range chiral imprinting of Cu(110) by tartaric acid,* T. J. Lawton, V. Pushkarev, D. Wei, F. R. Lucci, D. S. Sholl, A. J. Gellman, and E. C. H. Sykes, Journal of Physical Chemistry C, 117 (2013) 22290-22297
153. *Characterization of the thermodynamic stability of solvated metal-organic framework polymorphs using molecular simulations,* Jason A. Gee and David S. Sholl, Journal of Physical Chemistry C, 117 (2013) 20636-20642
154. *Signatures of normal and anomalous diffusion in nanotube systems by NMR,* M. Dvoyashkin, A. Wang, A. Katihar, J. Zang, G. I. Yuculen, S. Nair, D. S. Sholl, C. R. Bowers, and S. Vasenkov, Microporous and Mesoporous Materials, 178 (2013) 119-122
155. *Near surface phase transition of solute derived Pt monolayers,* Robert E. Rettew, Shuang Cheng, Marc Sauerbrey, Thomas A. Manz, David S. Sholl, Cherno Jaye, Daniel A. Fischer, and Faisal M. Alamgir, Topics in Catalysis, 56 (2013) 1065-1073
156. *Efficient and accurate methods for characterizing effects of framework flexibility on molecular diffusion in zeolites: CH_4 diffusion in eight member ring zeolites,* Rohan V. Awati, Peter I. Ravikovitch, and David S. Sholl, Journal of Physical Chemistry C, 117 (2013) 13462-13473
157. **MOF stability and gas adsorption as a function of exposure to water, humid air, SO_2, and NO_2,* Sangil Han, Yougui Huang, Taku Watanabe, Sankar Nair, Krista S. Walton, David S. Sholl, and J. Carson Meredith, Microporous and Mesoporous Materials, 173 (2013) 86-91
158. *Adsorption and diffusion of the Rh and Au adatom on graphene moire/Ru(0001),* Lymarie Semidey-Flecha, Dieh Teng, Bradley F. Habernicht, David S. Sholl, and Ye Xu, Journal of Chemical Physics, 138 (2013) 184710
159. **Surface interactions of C_2 and C_3 polyols with γ-Al_2O_3 and the role of coadsorbed water,* John R. Copeland, Xue-Rong Shi, David S. Sholl, and Carsten Sievers, Langmuir 29 (2013) 581-593
160. *Prediction of water adsorption in copper-based metal-organic frameworks using force fields derived from dispersion-corrected DFT calculations,* Ji Zang, Sankar Nair, and David S. Sholl, Journal of Physical Chemistry C, 117 (2013) 7519-7525
161. *On the relationship between Mo K edge energies and DFT computed partial charges,* Liwei Li, Michael R. Morrill, Heng Shou, David G. Barton, Daniela Ferrari, Robert J. Davis, Pradeep K. Agrawal, Christopher W. Jones, and David S. Sholl, J. Phys. Chem. C, 117 (2013) 2769-2773
162. **Adsorption and diffusion of small alcohols in zeolitic imidazolate frameworks ZIF-8 and ZIF-90,* Jason A. Gee, Jaeyub Chung, Sankar Nair, and David S. Sholl, J. Phys. Chem. C, 117 (2013) 3169-3176
163. *Thermodynamics of pore filling metal clusters in metal-organic frameworks: Pd in UiO-66,* Lasse B. Vilhelmsen and David S. Sholl, J. Phys. Chem. Lett., 3 (2012) 3702-3706
164. *First principles models of facilitating H_2 transport through metal films using spillover,* Shiqiang Hao and David S. Sholl, J. Phys. Chem. C, 117 (2013) 1217-1223
165. *First principles assessment of perovskite dopants for proton conductors with chemical stability and high conductivity,* Sung Gu Kang and David S. Sholl, RSC Advances, 3 (2013) 3333-3341

166. ***Rational tuning of water vapor and CO_2 adsorption in highly stable Zr-based MOFs,* H. Jasuja, Ji Zang, David S. Sholl, and Krista A. Walton, J. Phys. Chem. C 116 (2012) 23526-23532
167. *Rapid prediction of hydrogen permeation through amorphous metal membranes: An efficient computational screening approach,* Shiqiang Hao and David S. Sholl, Energy Env. Sci., 6 (2013) 232-240
168. *Use of infrared spectroscopy and density functional theory to study the influence of rubidium on alumina-supported molybdenum carbide catalyst for higher alcohol synthesis from syngas,* Heng Shou, Liwei Li, Daniela Ferrari, David S. Sholl, and Robert J. Davis, J. Catal., 299 (2013) 150-161
169. *Computationally efficient determination of hydrogen isotope effects on the thermodynamic stability of metal hydrides,* Kelly M. Nicholson and David S. Sholl, Phys. Rev. B, 86 (2012) 134113
170. *Quantifying large effects of framework flexibility on diffusion in MOFs: CH_4 and CO_2 in ZIF-8,* Emmanuel Haldoupis, Taku Watanabe, Sankar Nair, and David S. Sholl, ChemPhysChem, 13 (2012) 3449-3452
171. ***Accelerating applications of metal-organic frameworks for gas adsorption and separation by computational screening of materials,* Taku Watanabe and David S. Sholl, Langmuir, 28 (2012) 14114-14128 (feature article)
172. ***Improved atoms-in-molecule charge partitioning functional for simultaneously reproducing the electrostatic potential and chemical states in periodic and nonperiodic materials,* Thomas A. Manz and David S. Sholl, J. Chem. Theory Comput. 8 (2012) 2844-2867
173. ***Structure and mobility of metal clusters in MOFs: Au, Pd, and AuPd clusters in MOF-74,* Lasse B. Vilhelmsen, Krista A. Walton, and David S. Sholl, J. Am. Chem. Soc. 134 (2012) 12807-12816
174. **Analysis of equilibrium-based TSA processes for direct capture of CO_2 from air,* Ambarish Kulkarni and David S. Sholl, Ind. Eng. Chem. Res. 51 (2012) 8631-8645
175. **Identification of metal-organic framework materials for adsorption separation of rare gases: Applicability of Ideal Adsorbed Solution Theory (IAST) and effects of inaccessible framework regions,* Timothy van Heest, Stephanie L. Teich-McGoldrick, Jeffery A. Greathouse, Mark D. Allendorf, and David S. Sholl, J. Phys. Chem. C 116 (2012) 13183-13195
176. ***Prediction of CO_2 adsorption properties in zeolites using force fields derived from periodic dispersion-corrected DFT calculations,* Hanjun Fang, Preeti Kamakoti, Ji Zang, Stephen Cundy, Charanjit Paur, Peter I. Ravikovitch, and David S. Sholl, J. Phys. Chem. C, 116 (2012) 10692-10701
177. *Diffusion of tetrafluoromethane in single-walled aluminosilicate nanotubes: Pulsed field gradient NMR and molecular dynamics simulations,* M. Dvoyashkin, J. Zang, G. I. Yucelen, A. Katihar, S. Nair, D. S Sholl, C. R. Bowers, and S. Vasenkov, J. Phys. Chem. C, 116 (2012) 21350-21355
178. *Nucleation of Rh_n (n = 1-5) clusters on α-Al_2O_3 surfaces: Density functional theory study,* Xue-Rong Shi and David S. Sholl, J. Phys. Chem. C, 116 (2012) 10623-10631

179. ***Role of amine structure on CO_2 adsorption from ultra-dilute gas streams such as ambient air,* Stephanie A. Didas, Ambarish R. Kulkarni, David S. Sholl, and Christopher W. Jones, ChemSusChem, 5 (2012) 2058-2064
180. *Antiphase domain boundaries at the $Fe_3O_4(001)$ surface*, Gareth S. Parkinson, Thomas A. Manz, Zbynek Novotny, Phillip T. Sprunger, Richard L. Kurtz, Michael Schmid, David S. Sholl, and Ulrike Diebold, Phys. Rev. B, 85 (2012) 195450
181. ***Modification of the Mg/DOBDC MOF with Amines to Enhance CO_2 Adsorption from Ultradilute Gases,* Sunho Choi, Taku Watanabe, Tae-Hyun Bae, David S. Sholl, and Christopher W. Jones, J. Phys. Chem. Lett., 3 (2012) 1136-1141
182. ***Ultem/ZIF-8 Mixed Matrix Hollow Fiber Membranes for CO_2/N_2 Separations*, Ying Dai, J. R. Johnson, Oguz Karvan, David S. Sholl, and W. J. Koros, J. Membrane Science, 401-402 (2012) 76-82
183. **High-Throughput Screening of MOFs for CO_2 Separation*, Sangil Han, Yougui Huang, Taku Watanabe, Ying Dai, Krista S. Walton, Sankar Nair, David S. Sholl, and Carson Meredith, ACS Combi. Sci., 14 (2012) 263-267
184. ***Finding MOFs for Highly Selective CO_2/N_2 Adsorption Using Materials Screening Based on Efficient Assignment of Atomic Point Charges,* Emmanuel Haldoupis, Sankar Nair, and David S. Sholl, J. Am. Chem. Soc., 134 (2012) 4313-4323
185. **Single-Walled Aluminosilicate Nanotube/Poly(vinylalcohol) Nanocomposite Membranes*, D.-Y., Kang, H.-M. Tong, J. Zang, R. P. Choudhury, D. S. Sholl, H. W. Beckham, C. W. Jones, and S. Nair, ACS Applied Materials and Interfaces, 4 (2012) 965-976
186. *Predictions of sulfur resistance in metal membranes for H_2 purification using first-principles calculations,* Ki Chul Kim, Sung Gu Kang and David S. Sholl, Ind. Eng. Chem. Res., 51 (2012) 301-309
187. *Effect of TiH_2-induced strain on thermodynamics of hydrogen release from MgH_2,* Shiqiang Hao and David S. Sholl, J. Phys. Chem. C, 116 (2012) 2045-2050
188. *Identifying metal alloys with high hydrogen permeability using high throughput theory and experimental testing,* Sung Gu Kang, Kent E. Coulter, Sabina K. Gade, J. Douglas Way and David S. Sholl, J. Phys. Chem. Lett., **2** (2011) 3040-3044
189. **Methods for computing accurate atomic spin moments for collinear and noncollinear magnetism in periodic and nonperiodic materials*, Thomas A. Manz and David S. Sholl, J. Chemical Theory and Computation, **7** (2011) 4146-4164
190. *Examining the robustness of first-principles calculations for metal hydride thermodynamics by detection of metastable reaction pathways,* Ki Chul Kim, Anant Kulkarni, J. Karl Johnson and David S. Sholl, Phys. Chem. Chem. Phys., **13** (2011) 21520-21529
191. *Preparation and Gas Adsorption Characteristics of Zeolite MFI Crystals with Organic-Modified Interiors*, Mohamad H. Kassaee, David S. Sholl and Sankar Nair, J. Phys. Chem. C, **115** (2011) 19640-19646
192. *New fundamental experimental studies on α-$Mg(BH_4)_2$ and other borohydrides*, Hans Hagemann, Vincenza D'Anna, Jean-Phillipe Rapin, Radovan Cerny, Yaroslav Filinchuk, Ki Chul Kim, David S. Sholl, Stewart F. Parker, J. Alloys Compounds **509S** (2011) S688-S690

193. *Computational prediction of durable amorphous metal membranes for H_2 purification,* Shiqiang Hao and David S. Sholl, Journal of Membrane Science, **381** (2011) 192-196
194. *Sonochemical synthesis and characterization of sub-micron crystals of the metal-organic framework Cu[(hfipbb)(H_2hfipbb)$_{0.5}$]*, Cantwell G. Carson, Andrew J. Brown, David S. Sholl, and Sankar Nair, Crystal Growth and Design, **11** (2011) 4505-4510
195. *A porous maze,* David S. Sholl, Nature Chemistry **3** (2011) 429-430 [research highlight]
196. **Molecular simulations and theoretical predictions for adsorption and diffusion of CH_4/H_2 and CO_2/CH_4 mixtures in ZIFs,* Jinchen Liu, Seda Keskin, David S. Sholl, and J. Karl Johnson, J. Phys. Chem. C **115** (2011) 12560-12566
197. *Osmotic ensemble methods for predicting adsorption-induced structural transitions in nanoporous materials using molecular simulation,* Ji Zang, Sankar Nair and David S. Sholl, J. Chem. Phys. **134** (2011) 184103
198. *Chemical speciation of adsorbed glycine on metal surfaces,* Jeong Woo Han and David S. Sholl, J. Chem. Phys. **135** (2011) 034703
199. *Using First-principles Models to Advance Development of Metal Membranes for High Temperature Hydrogen Purification,* Sunggu Kang, Shiqiang Hao, and David S. Sholl, in Membrane Science and Technology vol. 14., S. Ted Oyama and Susan M. Stagg-Williams (eds.), Elsevier, Amsterdam, p. 309-331.
200. *Accurate treatment of electrostatics during molecular adsorption in nanoporous crystals without assigning point charges to framework atoms,* Taku Watanabe, Thomas A. Manz, and David S. Sholl, Journal of Physical Chemistry C, **115** (2011) 4824-4836
201. **Pore size analysis of > 250,000 hypothetical zeolites,* Emmanuel Haldoupis, Sankar Nair, and David Sholl, Physical Chemistry Chemical Physics, **13** (2011) 5053-5060.
202. *First principles screening of PdCuAg ternary alloys as H_2 purification membranes,* Chen Ling, Lymarie Semidey-Flecha, and David S. Sholl, J. Membrane Science, **371** (2011) 189-196
203. *Surface reactions of AsH_3, H_2Se, and H_2S on the Zn_2TiO_4(010) surface,* Shiqiang Hao, Rees B. Rankin, J. Karl Johnson, and David S. Sholl, Surface Science, **605** (2011) 818-823
204. *Large-scale screening of metal hydrides for hydrogen storage from first-principles calculations based on equilibrium reaction thermodynamics,* Ki Chul Kim, Anant D. Kulkarni, J. Karl Johnson, and David S. Sholl, Physical Chemistry Chemical Physics, **13** (2011) 7218-7229
205. *Density functional theory study of H and CO adsorption on K-promoted Mo_2C surfaces,* Jeong Woo Han, Liwei Li, and David S. Sholl, J. Physical Chemistry C, **115** (2011) 6870-6876
206. *$AZn_2(BH_4)_5$ (A = Li, Na) and $NaZn(BH_4)_3$: Structural Studies,* Radovan Cerny, Ki Chul Kim, Nicolas Penin, Vincenza D'Anna, Hans Hagemann, and David S. Sholl, J. Phys. Chem. C, **114** (2010) 19127-19133
207. *Role of Schottky defects in hydrogen and metal diffusion in NaH, MgH_2, and $NaMgH_3$,* Shiqiang Hao and David S. Sholl, J. Physical Chemistry Letters, **1** (2010) 2968-2973

208. *Predicting impurity gases and phases during hydrogen evolution from complex metal hydrides using free energy minimization enabled by first-principles calculations,* Ki Chul Kim, Mark D. Allendorf, Vitalie Stavila, and David S. Sholl, Physical Chemistry Chemical Physics, **12** (2010) 9918-9926
209. *First-principles characterization of amorphous phases of $MB_{12}H_{12}$, M = Mg, Ca,* Anant D. Kulkarni, Lin-Lin Wang, Duane D. Johnson, David S. Sholl, and J. Karl Johnson, J. Physical Chemistry C **114** (2010) 14601-14605
210. *Enantiospecific adsorption of amino acids on hydoxylated quartz (10-10),* Jeong Woo Han and David S. Sholl, Physical Chemistry Chemical Physics, 12 (2010) 8024-8032
211. *Predicting, fabricating, and permeability testing of free-standing ternary palladium-copper-gold membranes for hydrogen separation,* Kent E. Coulter, J. Douglas Way, Sabina K. Gade, Saurabh Chaudhari, David S. Sholl, and Lymarie Semidey-Flecha, Journal of Physical Chemistry C, **114** (2010) 17173-17180
212. ***Efficient calculation of diffusion limitations in metal organic framework materials: A tool for identifying materials for kinetic separations,* Emmanuel Haldoupis, Sankar Nair, and David S. Sholl, J. Am. Chem. Soc., **132** (2010) 7528-7539.
213. ***Chemically meaningful atomic charges that reproduce the electrostatic potential in periodic and nonperiodic systems,* Thomas Manz and David S. Sholl, J. Chem. Theory Comput., **6** (2010) 2455-2468.
214. *Detailed first-principles models of hydrogen permeation through PdCu-based ternary alloys,* Lymarie Semidey-Flecha, Chen Ling, and David S. Sholl, J. Membrane Sci., **362** (2010) 384-392.
215. **Molecular chemisorption on open metal sites in $Cu_3(BTC)_2$: A spatially periodic density functional theory study,* Taku Watanabe and David S. Sholl, J. Chem. Phys. **133** (2010) 094509
216. ***Can metal-organic framework materials play a useful role in large-scale carbon dioxide separations?* Seda Keskin, Timothy M. van Heest, and David S. Sholl, ChemSusChem, **3** (2010) 879-891.
217. *Chirality and rotation of surface-bound sulfides,* Heather L. Tierney, Jeong Woo Han, April. D. Jewell, Erin V. Iski, Ashleigh E. Baber, David S. Sholl, and E. Charles H. Sykes, J. Phys. Chem. C, **115** (2011) 897-901
218. *Flexibility of ordered hydroxyls influences the adsorption of molecules in single-walled aluminosilicate nanotubes,* Ji Zang, Shaji Chempath, Suchitra Konduri, Sankar Nair, and David S. Sholl, J. Phys. Chem. Lett., **1** (2010) 1235-1240
219. ***Selecting metal organic frameworks as enabling materials in mixed matrix membranes for high efficiency natural gas purification,* Seda Keskin and David S. Sholl, Energy & Environmental Science, **3** (2010) 343-351
220. *Comparison of first-principles calculations and experiments for hydrogen permeation through amorphous ZrNi and ZrNiNb films,* Shiqiang Hao and David S. Sholl, J. Membrane Sci. **350** (2010) 402-409
221. *The role of interstitial H_2 in hydrogen diffusion in light metal borohydrides*, Shiqiang Hao and David S. Sholl, Phys. Chem. Chem. Phys., **11** (2009) 11106-11109.

222. **Crystal structures and thermodynamic investigations of $LiK(BH_4)_2$, KBH_4, and $NaBH_4$ from first-principles calculations*, Ki Chul Kim and David S. Sholl, J. Phys. Chem. C, **114** (2010) 678-686
223. **Computational Identification of a Metal Organic Framework for High Selectivity Membrane-based CO_2/CH_4 Separations: $Cu(hfipbb)(H_2hfipbb)_{0.5}$,* Taku Watanabe, Seda Keskin, Sankar Nair, and David S. Sholl, Phys. Chem. Chem. Phys., **11** (2009) 11389-11394
224. *First principles evaluation of carbon diffusion in Pd and Pd-based alloys,* Chen Ling and David S. Sholl, Phys. Rev. B, **80** (2009) 214202.
225. *Self-diffusion and macroscopic diffusion of hydrogen in amorphous metals from first-principles calculations,* Shiqiang Hao and David S. Sholl, J. Chem. Phys. **130** (2009) 244705.
226. **Developing chiral surfaces for enantioselective chemical processing,* David S. Sholl and Andrew J. Gellman, AIChE J., 55 (2009) 2484-2490 [Highlighted in Chemical Engineering Progress, October 2009, p.16]
227. *Importance of kinetics in surface alloying: A comparison of the diffusion pathways of Pd and Ag atoms on Cu(111),* Darin O. Bellisario, Jeong Woo Han, Heather L. Tierney, Ashleigh E. Baber, David S. Sholl, and E. Charles H. Sykes, J. Phys. Chem. C, **113** (2009) 12863-12869
228. **Atomically detailed models of gas mixture diffusion through CuBTC membranes,* S. Keskin, J. Liu, J. Karl Johnson and David S. Sholl, Micro. Meso. Materials, **125** (2009) 101-106.
229. *A Dimensionless Reaction Coordinate for Quantifying the Lateness of Transition States,* Thomas A. Manz and David S. Sholl, Journal of Computational Chemistry, **31** (2010) 1528-1541.
230. ***Efficient methods for screening of metal organic framework membranes for gas separations using atomically-detailed models,* Seda Keskin and David S. Sholl, Langmuir, **25** (2009) 11786-11795.
231. *Enantiospecific adsorption of amino acids on hydroxylated quartz(0001),* Jeong Woo Han and David S. Sholl, Langmuir, **25** (2009) 10737-10745.
232. **Self diffusion of water and simple alcohols in single-walled aluminosilicate nanotubes,* Ji Zang, Suchitra Konduri, Sankar Nair, and David S. Sholl, ACS Nano, **3** (2009) 1548-1556
233. **Carbon dioxide and methane transport in DDR zeolite: insights from molecular simulations into carbon dioxide separations in small pore zeolites*, Sang Eun Jee and David S. Sholl, J. Am. Chem. Soc., **131** (2009) 7896-7904
234. *Selection of dopants to enhance hydrogen diffusion rates in MgH_2 and $NaMgH_3$,* Shiqiang Hao and David S. Sholl, Applied Physics Letters, **94** (2009) 171909.
235. ***Nanoscale design to enable the revolution in renewable energy,* Jason Baxter, Zhixi Bian, Gang Chen, David Danielson, Mildred S. Dresselhaus, Andrei G. Fedorov, Timothy S. Fisher, Christopher W. Jones, Edward Maginn, Uwe Kortshagen, Arumugam Manthiram, Arthur Nozik, Debra Rolison, Timothy Sands, Li Shi, David Sholl, and Yiyung Wu, Energy & Environmental Science, **2** (2009) 559-588.

236. *Probing hydrogen interactions with amorphous metals using first-principles calculations,* Shiqiang Hao, M. Widom, and David S. Sholl, J. Phys. Condens. Matter, **21** (2009) 115402.
237. *Step decoration of chiral metal surfaces*, Jeong Woo Han, John Kitchin, and David S. Sholl, J. Chemical Physics, **130** (2009) 124710.
238. *First principles investigation of metal sulfides as membranes in hydrogen purification,* Chen Ling and David S. Sholl, J. Membrane Science, **329** (2009) 153-159.
239. ***Assessing nanoparticle size effects on metal hydride thermodynamics using the Wulff construction,* Ki Chul Kim, Bing Dai, J. Karl Johnson, and David S. Sholl, Nanotechnology **20** (2009) 204001.
240. *Predictions of H isotope separation using crystalline and amorphous metal membranes: A computational approach*, Lymarie Semidey-Flecha, Shiqiang Hao, and David S. Sholl, J. Taiwan Inst. Chem. Eng. **40** (2009) 246-252 (invited paper for Ed Ma Festschrift)
241. **Hydrogen diffusion in MgH_2 and $NaMgH_3$ via concerted motions of charged defects,* Shiqiang Hao and David S. Sholl, Applied Physics Letters, 93 (2008) 251901
242. *Influence of surface reactions on complex hydride reversibility,* Bing Dai, Rees R. Rankin, J. Karl Johnson, Mark Allendorf, David S. Sholl, Nikolai A. Zarkevich, Duane D. Johnson, Journal of Physical Chemistry C, **112** (2008) 18270-18279.
243. ***Assessment of a metal-organic framework membrane for gas separations using atomically detailed calculations: CO_2, CH_4, N_2, H_2 mixtures in MOF-5,* Seda Keskin and David S. Sholl, Ind. Eng. Chem. Res. **48** (2009) 914-922.
244. *Using First-principles Calculations to Accelerate Materials Discovery for Hydrogen Purification Membranes by Modeling Amorphous Metals,* Shiqiang Hao and David S. Sholl, Energy and Environmental Science, **1** (2008) 175-183.
245. *The structure and reactivity of 2-butanol on Pd(111),* Feng Gao, Yilin Wang, Luke Burkholder, Carol Hirschmugl, Dilano Saldin, Hun Chuk Poon, David S. Sholl, Joanna N. James and Wilfred T. Tysoe, Surface Science, **602** (2008) 2264-2270.
246. *The real structure of naturally chiral Cu{643}*, Ashleigh E. Baber, Andrew J. Gellman, David S. Sholl, and E Charles H. Sykes, Journal of Physical Chemistry C, **112** (2008) 11086-11089.
247. *Atomistic simulations of CO_2 and N_2 diffusion in silica zeolites: The impact of pore size and shape,* David Selassie, Disan Davis, Jayme Dahlin, Eric Feise, Greg Haman, David S. Sholl, and Daniela Kohen, Journal of Physical Chemistry C, **112** (2008) 16521-16531.
248. ***Progress, opportunities, and challenges for applying atomically-detailed modeling to molecular adsorption and transport in metal-organic framework materials,* Seda Keskin, Jinchen Liu, Rees B. Rankin, J. Karl Johnson, and David S. Sholl, Industrial and Engineering Chemistry Research, **48** (2009) 2355-2371.
249. *Molecular simulations of hydrogen and methane permeation through pore mouth modified zeolite membranes*, Sang Eun Jee, Alan J. H. McGaughey, and David S. Sholl, Molecular Simulation, **35** (2009) 70-78.
250. **Testing the accuracy of correlations for multi-component mass transport of adsorbed gases in metal organic frameworks: Diffusion of CH_4/H_2 mixtures in*

CuBTC, Seda Keskin, Jinchen Liu, J. Karl Johnson, and David S. Sholl, Langmuir, **24** (2008) 8254.

251. *First principles calculations of methylamine and methanol adsorption on hydroxylated quartz (0001)*, Jeong Woo Han, Joanna N. James, and David S. Sholl, Surface Science, **602** (2008) 2478-2485.
252. **Combining Density Functional Theory and Cluster Expansion Methods to Predict H_2 Permeance Through Pd-based Binary Alloy Membranes*, Lymarie Semidey-Flecha and David S. Sholl, J. Chem. Phys., **128** (2008) 144701
253. *Large-scale screening of metal hydride mixtures for high-capacity hydrogen storage from first-principle calculations,* Sudhakar V. Alapati, J. Karl Johnson, and David S. Sholl, Journal of Physical Chemistry C, **112** (2008) 5258-5262
254. *Density functional theory studies of alloys in heterogeneous catalysis,* John R. Kitchin, Spencer D. Miller, and David S. Sholl, RSC Specialist Periodical Reports in Theoretical Chemistry, Chem. Modelling: Applications and Theory, **5** (2008) 150-181.
255. *DFT characterization of adsorption and diffusion mechanisms of H, As, S and Se on the zinc orthotitanate (010) surface*, Rees B. Rankin, Shiqiang Hao, David S. Sholl, and J. Karl Johnson, Surface Science, **602** (2008) 1877-1882.
256. **First principles study of experimental and hypothetical $Mg(BH_4)_2$ crystal structures*, Bing Dai, David S. Sholl, and J. Karl Johnson, J. Phys. Chem. C, **112** (2008) 4391-4395
257. *Density functional theory calculations of the surface structure of the inverse spinel zinc orthotitanate,* Rees B. Rankin, David S. Sholl, and J. Karl Johnson, J. Phys. Condensed Matt., **20** (2008) 095001
258. *Characterization of enantiospecific chemisorption on chiral Cu surfaces vicinal to Cu(111) and Cu(100) using Density Functional Theory,* Bhawna Bhatia and David S. Sholl, J. Chem. Phys., **128** (2008) 144709
259. *Characterization of bulk structure in zinc orthotitanate: a density functional theory and EXAFS investigation,* Rees B. Rankin, Andrew Campos, Hanjing Tian, Ranjani Siriwardane, Amitava Roy, James J. Spivey, David S. Sholl, and J. Karl Johnson, J. Am. Ceram. Soc., **91** (2008) 584-590.
260. ***Scalable fabrication of carbon nanotube/polymer nanocomposite membranes for high flux gas transport,* Sangil Kim, Joerg R. Jinschek, Haibin Chen, David S. Sholl, and Eva Marand, Nano Lett., **9** (2007) 2806-2811.
261. *The physico-chemical properties of cinchona alkaloids responsible for their unique performance in chiral catalysis,* Larry Mink, Zhen Ma, Ryan A. Olsen, Joanna James, David S. Sholl, Leonard J. Mueller, and Francisco Zaera, Topics in Catalysis, **48** (2008) 120-127
262. *Stability analysis of doped materials for reversible hydrogen storage in destabilized metal hydrides,* Sudhakar Alapati, J. Karl Johnson, and David S. Sholl, Phys. Rev. B, **76** (2007) 104108
263. **Theoretical studies of chiral adsorption on solid surfaces*, Joanna N. James and David S. Sholl, Current Opinions in Colloid and Interface Science **13** (2008) 60-64
264. *Using first-principles calculations to predict surface resistances to H_2 transport through metal alloy membranes*, Chen Ling and David S. Sholl, J. Membrane Sci., **303** (2007) 162

265. ***Screening metal-organic framework materials for membrane-based methane/carbon dioxide separations*, Seda Keskin and David S. Sholl, J. Phys. Chem. C, **111** (2007) 14055-14059
266. *Density Functional Theory studies of dehydrogenated and zwitterionic glycine and alanine on Pd and Cu surfaces,* Joanna N. James and David S. Sholl, J. Mol. Catal. A, **281** (2008) 44-48
267. *Density functional theory of β-hydride elimination of ethyl on flat and stepped Cu surfaces*, Xin Li, Andrew J. Gellman, and David S. Sholl, J. Chem. Phys., **127** (2007) 144710
268. **Experimental and Computational Prediction of the Hydrogen Transport Properties of Pd_4S*, Bryan D. Morreale, Bret H. Howard, Osemwengie Iyoha, Robert M. Enick, Chen Ling, and David S. Sholl, Ind. Eng. Chem. Res., **46** (2007) 6313-6319
269. *Soaking It All Up (book review),* David S. Sholl, Materials Today, **10** (2007) 61.
270. *Tuning Selectivity in Adsorption on Composite Chiral Surfaces,* Pawel Szabelski and David S. Sholl, J. Phys. Chem. C, 111 (2007) 11936-11942.
271. **Examining the accuracy of Ideal Adsorbed Solution Theory without curve-fitting using Transition Matrix Monte Carlo,* Haibin Chen and David S. Sholl, Langmuir, **23** (2007) 6431-6437.
272. *First principles investigation of adsorption and dissociation of hydrogen on Mg_2Si surfaces*, Bing Dai, David S. Sholl, and J. Karl Johnson, J. Phys. Chem. C, **111** (2007) 6910-6916.
273. *Brownian Dynamics simulations of copolymer-stabilized nanoparticles in the presence of an oil-water interface*, Abdulwahab S. Almusallam and David S. Sholl, J. Colloid Interface Sci., **313** (2007) 345-352
274. *Chiral separation on a model adsorbent with periodic surface heterogeneity,* Pawel Szabelski and David S. Sholl, J. Chem. Phys., **126** (2007) 144709.
275. ***Using first principles calculations to identify new destabilized metal hydride reactions for reversible storage,* Sudhakar V. Alapati, J. Karl Johnson, and David S. Sholl, Phys. Chem. Chem. Phys., **9** (2007) 1438-1452 (feature article)
276. *First principles screening of destabilized metal hydrides for high capacity H_2 storage using scandium*, Sudhakar V. Alapati, J. Karl Johnson, and David S. Sholl, J. Alloys Compounds, **446-447** (2007) 23-27.
277. **Using Density Functional Theory to Study Hydrogen Diffusion in Metals: A Brief Overview,* David S. Sholl, J. Alloys Compounds, **446-447** (2007) 462.
278. **Predicting reaction equilibria for destabilized metal hydride decomposition reactions for reversible hydrogen storage,* Sudhakar V. Alapati, J. Karl Johnson, and David S. Sholl, J. Phys. Chem. C, **111** (2007) 1584.
279. *Molecular Dynamics Simulations of Mass Transfer Resistance in Grain Boundaries of Twinned Zeolite Membranes,* David A. Newsome and David S. Sholl, J. Phys. Chem. B, **110** (2006) 22681-22689
280. **Influences of Interfacial Resistances on Gas Transport Through Carbon Nanotube Membranes,* David A. Newsome and David S. Sholl, Nano Letters, **6** (2006) 2150-2153.
281. *Structures of Dense Glycine and Alanine Adlayers on Chiral Cu(3,1,17) Surfaces*, Rees B. Rankin and David S. Sholl, Langmuir, **22** (2006) 8096-8103.

282. *Atomically-detailed Simulations of Surface Resistances to Transport of CH_4, CF_4, and C_2H_6 through Silicalite Membranes*, David A. Newsome and David S. Sholl, Micro. Meso. Materials, **107** (2008) 286-295
283. *Dense Metal Membranes for Production of High Purity Hydrogen*, David S. Sholl and Y. H. Ma, MRS Bulletin, 31 (2006) 770-773
284. ***Making High-Flux Membranes with Carbon Nanotubes,* David S. Sholl and J. Karl Johnson*,* Science, **312** (2006), 1003 [Perspective Article]
285. *Testing Predictions of Macroscopic Binary Diffusion Coefficients Using Lattice Models with Site Heterogeneity*, David S. Sholl*,* Langmuir, **22** (2006) 3707-3714
286. *Bromine Atom Diffusion on Stepped and Kinked Copper Surfaces*, D. M. Rampulla, A. J. Gellman and David. S. Sholl, Surface Science, **600** (2006) 2171-2177
287. *Applications of Density Functional Theory to Heterogeneous Catalysis,* David S. Sholl, Chemical Modelling: Applications and Theory, **4** (2006) 108-160
288. ***Understanding Macroscopic Diffusion of Adsorbed Molecules in Crystalline Nanoporous Materials via Atomistic Simulations*, David S. Sholl, Acc. Chem. Res., **39** (2006) 403-411.
289. ***Identification of Destabilized Metal Hydrides for Hydrogen Storage Using First Principles Calculations*, Sudhakar V. Alapati, J. Karl Johnson and David S. Sholl*,* J. Phys. Chem. B, **110** (2006) 8769
290. *First principles studies of chiral reconstructions of Cu(100) by adsorbed glycine and alanine,* Rees B. Rankin and David S. Sholl, J. Chem. Phys., **124** (2006) 074703
291. *Efficient simulation of binary adsorption isotherms using Transition Matrix Monte Carlo,* Haibin Chen and David S. Sholl, Langmuir, **22** (2006) 709-716
292. *Towards Computational Screening of Ternary Metal Alloys for Hydrogen Purification Membranes,* Preeti Kamakoti and David S. Sholl, J. Membrane Sci., **279** (2006) 94-99.
293. *Enantiospecific Chemisorption of Small Molecules on Intrinsically Chiral Cu Surfaces,* Bhawna Bhatia and David S. Sholl, Angew. Chemie Int. Ed., **44** (2005) 7761.
294. *First Principles Study of Adsorption and Dissociation of CO on W(111),* Liang Chen, David S. Sholl, and J. Karl Johnson, J. Phys. Chem. B, **110** (2006) 1344-1349.
295. *Pt Thin Films on the Polar $LaAlO_3$(100) Surface: A First-Principles Study*, Aravind Asthagiri and David Sholl, Phys. Rev. B, **73** (2006) 125432
296. *Using β-hydride elimination to test propositions for characterizing surface catalyzed reactions*, Xin Li, Andrew J. Gellman and David S. Sholl, Surf. Sci. Lett., **600** (2006) L25-L28.
297. ***Adsorption and diffusion of carbon dioxide and nitrogen through single walled carbon nanotube membranes,* Anastasios I. Skoulidas, David S. Sholl, and J. Karl Johnson, J. Chem. Phys., **124** (2006) 054708
298. ***Transport Diffusion of Gases Is Rapid In Flexible Carbon Nanotubes*, Haibin Chen, J. Karl Johnson and David S. Sholl, J. Phys. Chem. B, **110** (2006) 1971-1975
299. *Quantitative Assessment of Hydrogen Diffusion by Activated Hopping and Quantum Tunneling in Ordered Intermetallics*, Bhawna Bhatia and David S. Sholl, Phys. Rev. B, **72** (2005) 224302.

300. **Structures of Enantiopure and Racemic Glycine and Alanine Adlayers on Cu(110) and Cu(100) Surfaces*, Rees B. Rankin and David S. Sholl, J. Phys. Chem. B, **109** (2005) 16764-16773.
301. **Self Diffusion and Transport Diffusion of Light Gases in Metal Organic Framework Materials Assessed Using Molecular Dynamics Simulations*, Anastasios I. Skoulidas and David S. Sholl, J. Chem. Phys. B., **109** (2005) 15760-15768.
302. ***Prediction of hydrogen flux through sulfur tolerant binary alloy membranes,* Preeti Kamakoti, Bryan D. Morreale, Michael V. Ciocco, Bret H. Howard, Richard P. Killmeyer, Anthony V. Cugini, and David S. Sholl, Science, **307** (2005) 569-573.
303. *Structure and Binding Site of Acetate on Pd(111) Determined Using Density Functional Theory and Low Energy Electron Diffraction,* Joanna James, Dilano K. Saldin, T. Zheng, W. T. Tysoe, and David S. Sholl, Catalysis Today, **105** (2005) 74-77.
304. *Concentration Dependence of Transport Diffusion of Ethane in Silicalite: A Comparison Between Neutron Scattering Experiments and Atomically-Detailed Simulations*, Shang-Shan Chong, Herve Jobic, Marie Plazanet and David Sholl, Chem. Phys. Lett., **408** (2005) 157-161.
305. **Predictive Assessment of Surface Resistances in Zeolite Membranes Using Atomically-Detailed Models,* David A. Newsome and David S. Sholl, J. Phys. Chem. B, **109** (2005) 7237-7244.
306. ***Predictions of selectivity and flux for CH_4/H_2 separations using single walled carbon nanotubes as membranes,* Haibin Chen and David S. Sholl, J. Membrane Sci., **269** (2006) 152-160.
307. *Brownian Dynamics Study of Polymer-Stabilized Nanoparticles,* Abdulwahab Almusallam and David S. Sholl, Nanotechnology, **16** (2005) S409-S415.
308. **Comparisons of Diffusive and Viscous Contributions to Transport Coefficients of Light Gases in Single-Walled Carbon Nanotubes,* Suresh K. Bhatia, Haibin Chen, and David S. Sholl, Molecular Simulation, **31** (2005) 643-649.
309. *DFT Study of Pt adsorption on low index SrTiO3 surfaces: $SrTiO_3$ (100), $SrTiO_3$ (111), $SrTiO_3$ (110)*, Aravind Asthagiri and David S. Sholl, Surface Science, **581** (2005) 66-87.
310. **Chemisorption and Diffusion of Hydrogen on Flat and Stepped Nickel Surfaces*, Bhawna Bhatia and David Sholl, J. Chem. Phys., **122** (2005) 204707.
311. ***Enantioselective Separation on Naturally Chiral Surfaces*, Joshua D. Horvath, Anjanette Koritnik, Preeti Kamakoti, David S. Sholl, and Andrew J. Gellman, J. Am. Chem. Soc. **126** (2004) 14988-14994.
312. *Kinetics of H_2 desorption from C_{60},* S. A. FitzGerald, R. Hannachi, D. Sethna, M. Rinkoski, Kurt K. Sieber, and David S. Sholl, Phys. Rev. B, **71** (2005) 045415.
313. *The Structure of Formate Species on Pd(111) Calculated by Density Functional Theory and Determined Using Low Energy Electron Diffraction,* T. Zheng, D. Stacchiola, J. James, D. S. Sholl, and W. T. Tysoe, Surface Science, **574** (2005) 166-174.
314. **Structure of enantiopure and racemic alanine adlayers on Cu(110),* Rees B. Rankin and David S. Sholl, Surf. Sci. Lett. **574** (2005) L1-L8

315. *First-principles study of C adsorption, O adsorption, and CO dissociation on flat and stepped Ni surfaces,* Tao Li, Bhawna Bhatia, and David S. Sholl, J. Chem. Phys. **121** (2004) 10241-10249.
316. ***TCE Dechlorination Rates, Pathways, and Efficiency of Nanoscale Iron Particles with Different Properties,* Yueqiang Liu, Sara Majetich, Krzysztof Matyjaszewski, Robert D. Tilton, David S. Sholl, and Gregory V. Lowry, Env. Sci. & Tech., **39** (2005) 1338-1345.
317. **Ab initio based lattice gas modeling of interstitial hydrogen diffusion in CuPd alloys*, Preeti Kamakoti and David S. Sholl, Phys. Rev. B., **71** (2005) 014301.
318. *Multiscale Models of Sweep Gas and Porous Support Effects on Zeolite Membranes,* Anastasios I. Skoulidas and David S. Sholl, AIChE J., **51** (2005) 867-877.
319. *Diffusion of hydrogen in cubic Laves phase $HfTi_2H_x$,* Bhawna Bhatia, Xinjun Luo, C. A. Sholl, and David S. Sholl, J. Phys.:Condens. Matter. **16** (2004) 8891-8903
320. *Determination of concentration dependent transport diffusivity of CF_4 in silicalite by neutron scattering experiments and molecular dynamics simulations,* Hervé Jobic, Anastasios I. Skoulidas, and David S. Sholl, J. Phys. Chem. B, **108** (2004) 10613-10616.
321. *Orientation of ethoxy, mono-, di-, and tri-fluoroethoxy on Cu(111): A DFT study,* Xin Li, Andrew J. Gellman, and David S. Sholl, J. Mol. Catal. A, **228** (2005) 77-82.
322. *Titration of chiral kink sites on Cu(643) using Iodine adsorption,* Preeti Kamakoti, Joshua Horvath, Andrew J. Gellman, and David S. Sholl, Surf. Sci., **563** (2004) 206-216.
323. ***Rapid Diffusion of CH_4/H_2 Binary Mixtures in Carbon Nanotubes,* Haibin Chen and David S. Sholl, J. Am. Chem. Soc., **126** (2004) 7778-7779.
324. *Pt Thin Films on Stepped $SrTiO_3$ Surfaces: $SrTiO_3(620)$ and $SrTiO_3(622)$*, Aravind Asthagiri and David S. Sholl, J. Mol. Catal. A, **216** (2004) 233-246.
325. *Density Functional Theory Studies of the Interaction of H, S, Ni-H, and Ni-S, Complexes with MoS_2 Basal Plane,* Dan Sorescu, David S. Sholl, and Anthony V. Cugini, J. Phys. Chem. B, **108** (2004) 239-249
326. *Mechanisms and Rates of Interstitial H_2 Diffusion in Crystalline C_{60}*, Blas P. Uberuaga, Arthur F. Voter, Kurt Ken Sieber, and David S. Sholl, Physical Review Letters, **91** (2003) 105901.
327. ***Molecular Dynamics of self, corrected, and transport diffusivities of light gases in four silica zeolites to assess influences of pore shape and connectivity,* Anastasios I. Skoulidas and David S. Sholl, J. Phys. Chem. A, **107** (2003) 10132-10141.
328. ***Correlation effects in diffusion of CH_4/CF_4 mixtures in MFI zeolite. A study linking MD simulations with the Maxwell-Stefan formulation,* Anastasios I. Skoulidas, David S. Sholl, and R. Krishna, Langmuir, **19** (2003) 7977-7988.
329. **Density Functional Theory Studies of Sulfur Binding on Pd, Cu, Ag, and Their Alloys,* Dominic R. Alfonso, Anthony V. Cugini, and David S. Sholl, Surface Science, **546** (2003), 12-26.
330. *Comparing Atomistic Simulations and Experimental Measurements for CH_4/CF_4 Mixture Permeation Through Silicalite Membranes,* Anastasios I. Skoulidas, Travis C. Bowen, Christopher M. Doelling, John L. Falconer, Richard D. Noble, and David S. Sholl, Journal of Membrane Science, **227** (2003) 123-136.

331. **Assessment of Heterochiral and Homochiral Glycine Adlayers on Cu(110) Using Density Functional Theory,* Rees B. Rankin and David S. Sholl, Surface Science, **548** (2004), 301-308.
332. ***Chiral Selection on Inorganic Crystalline Surfaces,* Robert M. Hazen and David S. Sholl, Nature Materials **2** (2003) 367-374 (invited review article).
333. ***A Comparison of Hydrogen Diffusivities in Pd and CuPd Alloys Using Density Functional Theory,* Preeti Kamakoti and David S. Sholl, Journal of Membrane Science, **225** (2003) 145-154.
334. ***Monte Carlo Simulation of Single- and Binary-Component Adsorption of CO_2, N_2, and H_2 in Zeolite Na-4A,* E. Demet Akten, Ranjani Siriwardane, and David S. Sholl, Energy and Fuels, **17** (2003) 977-983.
335. ***Diffusivities of Ar and Ne in Carbon Nanotubes*, David M. Ackerman, Anastasios I. Skoulidas, David S. Sholl, and J. Karl Johnson, Molecular Simulation, **29** (2003), 677.
336. **Thin Pt films on the polar $SrTiO_3$(111) surface: an experimental and theoretical study*, Aravind Asthagiri, Christoph Niederberger, Andrew J. Francis, Lisa M. Porter, Paul A. Salvador, and David S. Sholl, Surface Science, **537** (2003) 367-364.
337. *A Comparative Study of CO Chemisorption on Flat and Stepped Ni Surfaces Using Density Functional Theory,* Vaishali Shah, Tao Li, Kenneth L. Baumert, Hansong Cheng, and David S. Sholl, Surface Science, **537** (2003) 217-227.
338. *Igniting Nanotubes With A Flash*, Bradley Bockrath, J. Karl Johnson, David S. Sholl, Bret Howard, Christopher Matranga, Wei Shi, and Daniel Sorescu, Science **297** (2002) 192 [non-peer reviewed letter].
339. ***Rapid Transport of Gases in Carbon Nanotubes*, Anastasios I. Skoulidas, David M. Ackerman, J. Karl Johnson, and David S. Sholl, Physical Review Letters, **89** (2002) 185901.
340. *Analysis of Binary Transport and Self-Diffusivities in a Lattice Model for Silicalite*, David Blanco Maceiras and David S. Sholl, Langmuir, **18** (2002) 7393-7400.
341. *First Principles Study of Adsorption and Diffusion of Ni and Ni-thiophene Complexes on MoS_2 Basal Planes*, Daniel Sorescu, David S. Sholl, and Anthony Cugini, J. Phys. Chem. B., **107** (2003) 1988-2000.
342. **Atomistic Simulations of CO_2 and N_2 Adsorption in Silica Zeolites: The Impact of Pore Size and Shape*, Anne Goj, David S. Sholl, E. Demet Akten, and Daniela Kohen, J. Phys. Chem. B, **106** (2002) 8367-8375.
343. **First Principles Study of Pt Adhesion and Growth on SrO- and TiO_2-terminated $SrTiO_3$(100),* Aravind Asthagiri and David S. Sholl, J. Chem. Phys., **116** (2002) 9914-9925.
344. **Can Chiral Single Walled Nanotubes Be Used As Enantiospecific Adsorbents?,* Timothy D. Power, Anastasios I. Skoulidas, and David S. Sholl, J. Am. Chem. Soc., **124** (2002) 1858-1859.
345. **Atomically Detailed Models of the Effect of Thermal Roughening on the Enantiospecificity of Naturally Chiral platinum Surfaces,* Timothy D. Power, Aravind Asthagiri, and David S. Sholl, Langmuir, **18** (2002) 3737-3748.

346. ***Transport Diffusivities of CH_4, CF_4, He, Ne, Ar, Xe, and SF_6 in Silicalite From Atomistic Simulations*, Anastasios I. Skoulidas and David S. Sholl, J. Phys. Chem. B., **106** (2002) 5058-5067.
347. ***Adsorption and Separation of Hydrogen Isotopes in Carbon Nanotubes: Multicomponent Grand Canonical Monte Carlo Simulations,* Sivakumar R. Challa, David S. Sholl, and J. Karl Johnson, Journal of Chemical Physics, **116** (2002) 814-824.
348. **A Comparison of Atomistic Simulations and Experimental Measurements of Light Gas Permeation Through Zeolite Membranes,* Travis C. Bowen, John L. Falconer, Richard D. Noble, Anastasios I. Skoulidas, and David S. Sholl, Industrial and Engineering Chemistry Research, **41** (2002) 1641-1650.
349. ***Direct Tests of the Darken Approximation for Molecular Diffusion in Zeolites Using Equilibrium Molecular Dynamics,* Anastasios I. Skoulidas and David S. Sholl, Journal of Physical Chemistry B, **105** (2001) 3151-3154.
350. ***Naturally Chiral Metal Surfaces as Enantiospecific Adsorbents,* David S. Sholl, Aravind Asthagiri, and Timothy D. Power, Journal of Physical Chemistry B, **105** (2001) 4771-4782 [invited feature article].
351. **Light Isotope Separation in Carbon Nanotubes Through Quantum Molecular Sieving,* Sivakumar R. Challa, David S. Sholl, and J. Karl Johnson, Physical Review B, **63** (2001) 245419.
352. *Thermal Fluctuations in the Structure of Naturally Chiral Pt Surfaces,* Aravind Asthagiri, Peter J. Feibelman, and David S. Sholl, Topics in Catalysis, **18** (2002) 193-200.
353. *Effects of Surface Relaxation on Enantiospecific Adsorption on Naturally Chiral Pt Surfaces,* Timothy D. Power and David S. Sholl, Topics in Catalysis, **18** (2002) 201-208.
354. *Predicting Single-Component Permeance Through Macroscopic Zeolite Membranes from Atomistic Simulations*, David S. Sholl, Industrial and Engineering Chemistry Research, **39** (2000) 3737.
355. *Brownian Dynamics Simulation of the Motion of a Rigid Sphere in a Viscous Fluid Very Near A Wall*, David S. Sholl, Michael K. Fenwick, Edward Atman, and Dennis C. Prieve, Journal of Chemical Physics, **113** (2000) 9268.
356. *Kinetics of Hard Sphere and Chain Adsorption into Circular and Elliptical Pores*, Anastasios I. Skoulidas and David S. Sholl, Journal of Chemical Physics, **113** (2000) 4379.
357. *Enantiospecific Properties of Chiral Single Crystal Surfaces*, Joshua D. Horvath, Andrew J. Gellman, David S. Sholl, and Timothy D. Power, in "*Chirality: Physical Chemistry*", Janice Hicks (ed.), ACS Symposium Series, **810** (2002) 269-282.
358. *Influences of Concerted Cluster Diffusion on Single File Diffusion of CF_4 in $AlPO_4$-5 and Xe in $AlPO_4$-31,* David S. Sholl and Cha Kun Lee, Journal of Chemical Physics, **112** (2000) 817.
359. *Modeling Single-Component Permeation Through A Zeolite Membrane from Atomic-scale Principles,* David S. Sholl, in "Nanoporous Materials II", A Sayari, M. Jaroniec, and T. Pinnavia (eds.). Elsevier, Amsterdam (2000).
360. ***Quantum Sieving in Carbon Nanotubes and Zeolites,* Qinyu Wang, Sivakumar Challa, David S. Sholl, and J. Karl Johnson, Physical Review Letters **82** (1999) 956.

361. *Characterization of Molecular Cluster Diffusion in $AlPO_4$-5 Using Molecular Dynamics,* David S. Sholl, Chemical Physics Letters, **305** (1999) 269.
362. *Characterizing Adsorbate Passage in Molecular Sieve Pores,* David S. Sholl, Chemical Engineering Journal, **74** (1999) 25.
363. *Enantiospecific Adsorption of Chiral Hydrocarbons on Naturally Chiral Pt and Cu Surfaces,* Timothy D. Power and David S. Sholl, Journal of Vacuum Science and Technology A, **17** (1999) 1700.
364. ***A Generalized Surface Hopping Model*, David S. Sholl and John C. Tully, Journal of Chemical Physics **109** (1998) 7702.
365. *Reply to Comment on "Normal, Single-File, and Dual-Mode Diffusion of Binary Adsorbate Mixtures in $AlPO_4$-5"*, David S. Sholl and Kristen A. Fichthorn, Journal of Chemical Physics **109** (1998) 5693.
366. ***Adsorption of Chiral Hydrocarbons on Chiral Platinum Surfaces,* David S. Sholl, Langmuir, **14** (1998) 862.
367. **Concerted Diffusion of Molecular Clusters in a Molecular Sieve*, David S. Sholl and Kristen A. Fichthorn, Physical Review Letters **79** (1997) 3569.
368. **Normal, Single-File, and Dual-Mode Diffusion of Binary Adsorbate Mixtures in $AlPO_4$-5*, David S. Sholl and Kristen A. Fichthorn, Journal of Chemical Physics **107** (1997) 4384.
369. *Molecular Dynamics of Adsorption and Diffusion of* n-*Butane Adlayers on Pt(111)*, Janhavi S. Raut, David S. Sholl and Kristen A. Fichthorn, Surface Science **389** (1997) 88.
370. *Adsorption Kinetics of Chemisorption by Surface Abstraction and Dissociative Adsorption*, David S. Sholl, Journal of Chemical Physics **106** (1997) 289.
371. *The Effect of Correlated Flights in Particle Mobilities During Single-File Diffusion*, David S. Sholl and Kristen A. Fichthorn, Physical Review E **55** (1997) 7753.
372. *The Influence of Cluster Diffusion on the Coarsening of Xe Films on Pt(111)*, David S. Sholl, Kristen A. Fichthorn, and Rex T. Skodje, Journal of Vacuum Science and Technology A **15** (1997) 1275.
373. *Comment on 'Constant Temperature Molecular Dynamics by Means of a Stochastic Collision Model II: The Harmonic Oscillator'[J. Chem. Phys. 104 (1996) 3732]*, David S. Sholl and Kristen A. Fichthorn, Journal of Chemical Physics **106** (1997) 1646.
374. **Late Stage Coarsening of Adlayers by Dynamic Cluster Coalescence*, David S. Sholl and Rex T. Skodje, Physica A **231** (1996) 631.
375. *A Model Surface Reaction on Stepped Surfaces*, David S. Sholl and Rex T. Skodje, Surface Science **345** (1996) 173.
376. ***Diffusion of Clusters of Atoms and Vacancies on Surfaces and the Dynamics of Diffusion Driven Cluster Coarsening*, David S. Sholl and Rex T. Skodje, Physical Review Letters **75** (1995) 3158.
377. *Exact Solutions of the Monomer-Monomer Reaction: Segregation, Poisoning, and Interface Evolution*, David S. Sholl and Rex T. Skodje, Physical Review E **53** (1995) 335.

378. *Surface Diffusion of H and CO on Cu/Ru(001): Evidence for Long-Range Trapping by Copper Islands*, David E. Brown, David S. Sholl, Rex T. Skodje, and Steven M. George, Chemical Physics **201** (1995) 273.
379. *Kinetic Phase Transitions and Bistability in a Model Surface Reaction I: Monte Carlo Simulations*, David S. Sholl and Rex T. Skodje, Surface Science **334** (1995) 295.
380. *Kinetic Phase Transitions and Bistability in a Model Surface Reaction II: Spatially Inhomogeneous Theories*, David S. Sholl and Rex T. Skodje, Surface Science **334** (1995) 305.
381. *Comment on 'A Theoretical Stochastic Model for the* $A+1/2B_2 \rightarrow 0$ *Reaction [J. Chem. Phys. 98 (1993) 10017]*, David S. Sholl and Rex T. Skodje, Journal of Chemical Physics **101** (1994) 855.
382. *Diffusion of Xenon on a Platinum Surface: The Influence of Correlated Flights*, David S. Sholl and Rex T. Skodje, Physica D **71** (1994) 168.
383. *Optimal Resolution in Maximum Entropy Image Reconstruction from Projections with Multigrid Acceleration*, Mark A. Limber, Tom A. Manteuffel, Stephen F. McCormick, and David S. Sholl, Proc. Of the Sixth Copper Mountain Conference on Multigrid Methods (1993) 361.
384. *A Semi-Lagrangian Approach to the Shallow Water Equations*, J. R. Bates, Stephen F. McCormick, John Ruge, David S. Sholl, and Irad Yavneh Proc. Of the Sixth Copper Mountain Conference on Multigrid Methods (1993) 593.
385. *Perturbative Calculation of Superperiod Recurrence Times in Nonlinear Chains*, David S. Sholl and B. I. Henry, Physics Letters A **159** (1991) 21.
386. *Recurrence Times in Cubic and Quartic Fermi-Pasta-Ulam Chains: A Shifted-Frequency Analysis*, David S. Sholl and B. I. Henry, Physical Review A **44** (1991) 6364.
387. *Modal Coupling in One-Dimensional Anharmonic Chains*, David S. Sholl, Physics Letters A **149** (1990) 253.

Books

Non-fiction

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

- Turkish edition published in 2014.
- Japanese and Chinese editions published in 2015.
- > 1500 citations reported by Google Scholar.

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
4. Adsorbent materials and methods of adsorbing carbon dioxide, P. I. Ravikovitch, D. Sholl, C. Paur, K. G. Strohmaier, H. Fang, A. R. Kulkarni, R. V. Awati, P. Kamakoti, US Patent 10,744,449, Issued August 18, 2020

Departmental Seminars and Invited Presentations

1. Chemical Engineering Alumni Lectures, University of Massachusetts Amherst, September 2021
2. Symposium on Surface Chemistry and Solvation Effects in Confined Environments, ACS Virtual National Meeting, April 2021
3. Virtual seminar, International Adsorption Society, March 2021
4. Plenary talk, North American Membrane Society 2020 Meeting (virtual meeting), May 2020
5. Department of Chemical and Environmental Engineering, University of Arizona, Tucson, AZ, October 2019
6. Doumas Lecture in Chemical Engineering, Department of Chemical Engineering, Virginia Tech, Blacksburg, VA, October 2019
7. Reproducibility in Science and Engineering, ACS 66th International Symposium, Columbus, OH, October 2019
8. Department of Chemical Engineering, Seoul National University, Seoul, South Korea, October 2019
9. Department of Chemical Engineering, Nanyang University, Singapore, October 2019
10. Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, October 2019
11. Department of Chemical and Biomolecular Engineering, University of Notre Dame, South Bend, IN, September 2019
12. Keynote Lecture, DOE BES Separations PI Meeting, Gaithersburg, MD, September 2019
13. School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ, September 2019
14. School of Chemical & Biomolecular Engineering, Georgia Tech, August 2019
15. Gordon Research Conference on Nanoporous Materials, Andover, NH, August 2019
16. Department of Chemical Engineering, New Mexico State University, Las Cruces, NM, April 2019
17. Department of Chemical Engineering, University of Arkansas, April 2019
18. Symposium on New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations and Theory, ACS National Meeting, Orlando, FL, March 2019
19. George Olah Award Symposium in Honor of Chunshan Song, ACS National Meeting, Orlando, FL, March 2019

20. Department of Chemical Engineering, University of New Hampshire, Durham, NH, March 2019
21. Ma Lecture, Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA, March 2019
22. Physical Sciences Division, Pacific Northwest National Laboratory, Richland, WA, March 2019
23. Department of Chemical Engineering, Oklahoma State University, Stillwater, OK, December 2018
24. University College London, London, UK, December 2018
25. Department of Chemical Engineering, Virginia Commonwealth University, Richmond, VA, October 2018
26. Department of Chemical Engineering, Drexel University, Philadelphia, PA, November 2018
27. Department of Chemical Engineering and Materials Science, University of Alberta, Edmonton, Alberta, October 2018
28. Parr Lecture, Department of Chemical and Biomolecular Engineering, University of Illinois, Champaign, IL, September 2018
29. Plenary Lecture, 15th International Conference on Inorganic Membranes, Dresden, Germany, June 2018
30. Department of Nanoengineering, UCSD, La Jolla, CA, April 2018
31. Department of Chemical Engineering, UC Berkeley, Berkeley, CA, March 2018
32. Department of Chemical Engineering, South Dakota School of Mines, March 2018
33. Plenary Lecture, 2018 US DOE Basic Energy Sciences Separation Science PI Meeting, Gaithersburg, MD, February 2018
34. Material Informatics Seminar, National Institute of Standards, Gaithersburg, MD, February 2018
35. New Vistas in Molecular Thermodynamics, Humboldt Kolleg, Berkeley, CA, January 2018
36. NAS Committee on Reproducibility and Replicability in Science, Washington DC, December 2017
37. Sustainable Engineering Forum Plenary Session, AIChE Annual Meeting, Minneapolis, MN, November 2017
38. Department of Chemical Engineering, MIT, Boston, MA, October 2017
39. Department of Chemical Engineering, Tulane University, New Orleans, LA, September 2017
40. Department of Chemical Engineering, Kansas State University, Manhattan, KS, September 2017
41. Department of Chemical & Petroleum Engineering, University of Kansas, Lawrence, KS, September 2017
42. Sandia National Laboratory, Albuquerque, NM, August 2017
43. ORNL Materials Informatics Workshop, Oak Ridge National Lab, Oak Ridge, TN, August 2017
44. ASEE Summer School for Chemical Engineering Faculty, Raleigh, NC, August 2017
45. Keynote Lecture, Australian CCS Research Conference, Melbourne, VIC, Australia, June 2017

46. AINST Distinguished Seminar, University of Sydney, Sydney, NSW, Australia, June 2017
47. Department of Chemical Engineering, University of New South Wales, Kensington, NSW, Australia, June 2017
48. Department of Physics Colloquium, University of Queensland, Brisbane, QLD, Australia, June 2017
49. CSIRO and University of Monash Department of Chemistry, Clayton, VIC, Australia, May 2017
50. Mieyungah Public Lecture, University of Melbourne, Melbourne, Australia, May 2017
51. Tau Beta Pi Initiates Dinner talk, Georgia Institute of Technology, Atlanta, GA, April 2017
52. Department of Chemical Engineering, University of California Davis, Davis, CA, March 2017
53. Department of Chemical Engineering, Colorado School of Mines, Golden, CO, January 2017
54. Robin H. Stokes Lecture, University of New England, Armidale, NSW, Australia, December 2016
55. Plenary Lecture, Fundamentals and Applications of Advanced Porous Materials Conference, Adelaide, South Australia, Australia, December 2016
56. Department of Chemical and Biological Engineering, University of Delaware, Newark, DE, December 2016
57. Department of Chemical Engineering and Materials Science, Cal Poly Pomona, Pomona, CA, November 2016
58. Department of Chemical Engineering, Texas Tech, Lubbock, TX, November 2016.
59. Georgia Research Alliance Eminent Scholars Annual Meeting, Atlanta, GA, October 2016.
60. Symposium on Supramolecular Assemblies and Metal-Organic Frameworks, SERMACS, Columbia, SC, October 2016.
61. University of Houston Honors College, Houston, TX, October 2016
62. School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, September 2016
63. Department of Chemical Engineering, University College Dublin, Dublin, Ireland, September 2016
64. International Zeolite Membrane Meeting 2016, Dalian, China, August 2016
65. University of Seoul, Seoul, Korea, August 2016
66. Seoul National University, Seoul, Korea, August 2016
67. Board for Chemical Sciences and Technology, National Academy of Sciences, Irvine, CA, August 2016.
68. Gordon Conference on Membranes, New London, NH, August 2016.
69. Gulf Coast and Latin America Scientists Association Seminar Series, Dow Chemical, Freeport, TX, May 2016
70. Savannah River National Laboratory, Aiken, SC, May 2016
71. Symposium on Design, Synthesis and Applications of Advanced Porous Materials, Pacifichem, Honolulu, HI, December 2015

72. Symposium on Data Mining and Machine Learning Meets Experiment and First-principles Simulation for Materials Discovery, Pacifichem, Honolulu, HI, December 2015
73. Symposium on Safety in the Academic Research Laboratory, Pacifichem, Honolulu, HI, December 2015
74. Department of Chemical, Petroleum and Materials Engineering, University of Southern California, Los Angeles, CA, October 2015
75. Department of Chemical and Biomolecular Engineering, University of California Riverside, Riverside, CA, October 2015
76. Department of Chemical and Biomolecular Engineering, University of California Irvine, Irvine, CA, October 2015
77. Department of Chemical Engineering, University of Houston, Houston, TX, October 2015
78. Department of Chemical and Biomolecular Engineering, University of Florida, Gainesville, FL, September 2015
79. Department of Chemical and Biological Engineering, University of Buffalo, Buffalo, NY, September 2015
80. Department of Chemical Engineering, Northeastern University, Boston, MA, August 2015
81. Multiscale Porosity From Laboratory To Industrial Application, 2nd Micromeritics Workshop, Massachusetts Institute of Technology, Cambridge, MA, August 2015
82. School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, August 2015
83. US-Korea Conference on Science, Technology, and Entrepreneurship , Atlanta, GA, July 2015
84. DOE BES Catalysis Contractors Workshop, Annapolis, MD, July 2015
85. Gordon Research Conference on Hydrogen Metal Systems, Stonehill College, MA, July 2015
86. Workshop on Metal-Organic Frameworks, Telluride Scientific Research Conference, Telluride, CO, June 2015.
87. CECAM Workshop on Defects and Disorder in Metal-Organic Frameworks, Chimie ParisTech, Paris, France, June 2015
88. 3M Tech Talk, Minneapolis, MN, May 2015
89. UOP Technical Seminar, Des Plaines, IL, May 2015
90. Department of Chemical Engineering, University of Illinois at Chicago, Chicago, IL, May 2015
91. Symposium on Genomic Approaches to Materials, 249th ACS National Meeting, Denver, CO, March 2015
92. Symposium on Environmental Applications of Metal-Organic Frameworks, 249th ACS National Meeting, Denver, CO, March 2015
93. Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, March 2015
94. Department of Chemical and Biomolecular Engineering, University of South Florida, Tampa, FL, February 2015
95. Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD, December 2014

96. Chinese American Chemical Society Banquet, Atlanta, GA, November 2014
97. Molecular Thermodynamics Plenary Session, AIChE Annual Meeting, Atlanta, GA, November 2014
98. Fossil Fuels Plenary Session, AIChE Annual Meeting, Atlanta, GA, November 2014
99. Department of Chemical and Biomolecular Engineering, Columbia University, New York, NY, November 2014
100. Adsorption Technologies Group, Sasol, Sasolburg, South Africa, November 2014
101. Particle Technology Workshop, University of Cape Town, Cape Town, South Africa, November 2014
102. ExxonMobil Applied Materials Symposium, Hershey, PA, October 2014
103. Department of Chemical and Biomolecular Engineering, University of Colorado, Boulder, CO, October 2014
104. Trotter Distinguished Lecture, Department of Chemical Engineering, University of Tennessee, October 2014
105. Symposium on MOFs for Applications, 248th ACS National Meeting, San Francisco, CA, August 2014
106. School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, August 2014
107. Metal Hydrogen 2014, Manchester, UK, July 2014
108. Department of Chemical Engineering, Imperial College London, London, UK, July 2014
109. Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, July 2014
110. Department of Chemistry, National University of Singapore, Singapore, July 2014
111. Department of Chemical Engineering, University of Melbourne, Melbourne, Australia, June 2014
112. International Conference on Inorganic Membranes (keynote address), Brisbane, Australia, June 2014
113. MRS Spring Meeting, San Francisco, CA, April 2014
114. Florida AVS Meeting, Orlando, FL, March 2014
115. J. H. Hopps 5th Annual Training Symposium, Morehouse College, Atlanta, GA, February 2014
116. Dow Chemical Company, Freeport, TX, January 2014
117. School of Chemistry Colloquium, Georgia Institute of Technology, Atlanta, GA, October 2013
118. Physical Chemistry Seminar, University of Wisconsin, Madison, WI, October 2013
119. Department of Chemical and Biomolecular Engineering, Northwestern University, Evanston, IL, October 2013
120. International Zeolite Membrane Meeting, Jeju Island, South Korea, June 2013
121. Workshop on Adsorption in Compliant Solids, Paris, France, June 2013
122. International Conference on Energy and Sustainability, Hang Zhou, China, May 2013
123. Department of Physics, Oberlin College, Oberlin, OH, May 2013
124. Symposium on CO_2 Capture and Utilization, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013

125. Symposium on Hydrogen Production, Storage, and Utilization, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013
126. Symposium on Identification of Environmental Abiotic and Biotic Reactions Using Computational Chemistry, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013
127. Department of Chemistry, University of Florida, February 2013
128. Georgia Tech Clean Energy Speaker Series, Atlanta, GA, February 2013
129. CSIRO, Clayton, Victoria, Australia, December 2012
130. Dept. of Chemical Engineering, University of Queensland, December 2012
131. Pacific Northwest National Laboratory, December 2012
132. Department of Chemical Engineering, Clemson University, November 2012
133. Physical Chemistry seminar, Department of Chemistry, University College London, London, UK, October 2012
134. Air Capture: Developing Technologies for Carbon Recycling and Negative Emissions, Institution of Mechanical Engineering, London, UK, October 2012
135. MOF2012 Keynote Lecture, Edinburgh, UK, September 2012
136. Foundations of Molecular Modeling and Simulations, Portland, OR, July 2012.
137. NETL ORD Seminar, National Energy Technology Laboratory, Pittsburgh, PA, June 2012.
138. Symposium on Gas Capture Materials, Canadian Society of Chemistry Conference, Calgary, AB, May 2012
139. CNMS Theory Seminar, Oak Ridge National Laboratory, Oak Ridge, TN, May 2012
140. ORNL Reactor Off Gas Group, Oak Ridge National Laboratory, Oak Ridge, TN, May 2012
141. Washington University in St. Louis, Department of Energy, Environment, and Chemical Engineering, April 2012
142. University of South Carolina, Department of Chemical Engineering, Columbia, SC, March 2012
143. Materials Modeling Group, Intel Corporation, Santa Clara, CA, March 2012
144. Symposium on Non-adiabatic Dynamics: Surface Hopping and Beyond (invited talk), 243rd ACS National Meeting, San Diego, CA, March 2012
145. Symposium on High-Throughput Screening Approaches for Catalysts Discovery and Optimization (invited talk), 243rd ACS National Meeting, San Diego, CA, March 2012
146. University of California Berkeley, Carbon Capture Program, February 2012
147. Stanford University, Department of Energy Resources Engineering, February 2012
148. MADE@GT Symposium on Materials Design, Atlanta, GA, November, 2011
149. Georgia Research Alliance Eminent Scholars Annual Meeting, Atlanta, GA, October 2011
150. Department of Chemical Engineering Seminar, University of Kentucky, Louisville, KY, October 2011.
151. Sandia National Laboratory, Microfluidics Department, Livermore, CA, September 2011.

152. Nanoporous Materials VI (plenary presentation), Banff, Canada, August 21-24, 2011.
153. National Summit on Advancing Clean Energy Technologies (invited panelist), Washington DC, May 2011.
154. Workshop on Materials Design in Chemical Compound Space, Institute for Pure and Applied Mathematics, UCLA, Los Angeles, CA, May 2011
155. Symposium on Applications of Metal-Organic Frameworks, MRS Spring Meeting, San Francisco, CA, April 2011
156. APS March Meeting, Dallas, TX, March 2011
157. Department of Chemical Engineering, National University of Singapore, Singapore, February 2011
158. Institute for Atom-efficient Chemical Transformations Workshop, Northwestern University, Evanston, IL, November 2010
159. COMSEF Plenary Session, AIChE Annual Meeting, Salt Lake City, November 2010
160. Open Forum of the Energy and Environment, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, October 2010
161. Neutrons in Catalysis Workshop, Oak Ridge National Laboratory, September 2010
162. Symposium on Nanoporous Materials for Environmental Applications, ACS National Meeting, Boston, August 2010
163. 5th International Zeolite Membrane Meeting, Loutraki, Greece, May 2010.
164. Department of Chemical and Bioengineering, University of Washington, Seattle, WA, May 2010.
165. Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, April 2010.
166. Department of Chemical Engineering, The Pennsylvania State University, State College, PA, April 2010.
167. Keynote Lecture, Symposium on Advances in Membrane Science and Technology, ACS National Meeting, San Francisco, March 2010.
168. Dept. of Chemical Engineering, Texas A&M University, College Station, TX, January 2010.
169. Oak Ridge National Laboratory, Computational Materials Division, Knoxville, TN, January 2010.
170. Thin Films Division, AVS 56th International Symposium, San Jose, November 2009.
171. Dept. of Chemical Engineering, Clemson University, October 2009.
172. DOE Computational Materials Science Network Workshop, Denver, CO, October, 2009.
173. XVIII International Materials Research Congress, Cancun, Mexico, August 2009.
174. US-China Workshop on Surface Science and Heterogeneous Catalysis, Dalian, China, June 2009.
175. Savannah River National Laboratory, Materials Division, Aiken, SC, June 2009.
176. Swedish-American Entrepeneurial Days, Keynote Address, Savannah, GA, April 2009.

177. Emerson Center Annual Symposium, Emory University, March 2009.
178. Dept. of Chemical Engineering, University of Louisville, Louisville, KY, February 2009
179. Center for Simulational Physics, 22nd Annual Workshop, University of Georgia, Athens, GA, February 2009
180. Dept. of Chemical Engineering, University of New South Wales, Sydney , NSW, Australia, December 2008.
181. Dept. of Physics, University of Sydney, Sydney, NSW, Australia, December 2008.
182. Dept of Chemical Engineering, University of Melbourne, Melbourne, Victoria, Australia, December 2008
183. CSIRO Energy Research Center, Brisbane, Queensland, Australia, December 2008
184. Future Directions in Transport, Centennial Symposium, AIChE Annual Meeting, Philadelphia, November 2008.
185. Department of Chemical Engineering, University of Maine, Bangor, ME, October 2008
186. University of Queensland Physics Summer School, Stradbroke Island, Queensland, Australia, December 2008.
187. Center for Nanoscale Materials, Argonne National Laboratory, Chicago, IL, October 2008
188. Center for Simulational Physics, University of Georgia, Athens, GA, October 2008
189. College of Engineering, Peking University, Beijing, China, May 2008.
190. Department of Chemistry, Tsinghua University, Beijing, China, May 2008.
191. Department of Chemical Engineering, Beijing University of Chemical Technology, Beijing, China, May 2008.
192. Department of Chemistry, Emory University, Atlanta, GA, April 2008.
193. Thermodynamics in Chemical Engineering: Prospects and Perspectives, AIChE Spring Meeting, New Orleans, LA, April 2008.
194. Computational Methods and Molecular Modeling in Fuel Chemistry, ACS National Meeting, New Orleans, LA, April 2008.
195. Arthur W. Adamson Award for Distinguished Service of Surface Chemistry: Symposium in Honor of Francisco Zaera, ACS National Meeting, New Orleans, LA, April 2008.
196. Department of Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ, November 2007.
197. Department of Materials Science and Engineering, University of Illinois, Champaign, IL, November 2007.
198. MESD Plenary Session, AIChE Annual Meeting, Salt Lake City, UT, November 2007.
199. CECAM Workshop on Chirality at Surfaces, Lyons, France, October 2007.
200. Symposium on Advanced Materials for Conversion and Separations in Energy Applications, ACS National Meeting, Boston, MA, August 2007.
201. Symposium on Hydrogen Storage and Fuel Cell Technology, ACS National Meeting, Boston, MA, August 2007.

202. Gordon Conference on Hydrogen in Metals, Waterville, Maine, July 10, 2007.
203. Department of Chemical Engineering, Oklahoma University, April 19, 2007
204. Symposium on Capturing Complexity in Physical Sciences Simulation, ACS National Meeting, Chicago, IL, March 27, 2007
205. Symposium on Implications and Applications of Chirality in Physical Chemistry, ACS National Meeting, Chicago, IL, March 28, 2007
206. Department of Chemical Engineering and Materials Science, University of Minnesota, January 23, 2007.
207. Department of Chemistry, Carleton College, January 12, 2007.
208. Biosecurity and Nanosciences Laboratory, Lawrence Livermore National Laboratory, January 10, 2007.
209. COMSEF Plenary Session, AIChE Annual Meeting, San Francisco, California, November 12-16, 2006
210. Department of Chemical Engineering, Carnegie Mellon University, November 2, 2006
211. Department of Chemical Engineering, Vanderbilt University, October 30, 2006.
212. Department of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia, October 18, 2006
213. Metal-Hydrogen 2006, Maui, Hawaii, October 1-6, 2006
214. Symposium on Challenges for the Hydrogen Economy: Storage Science and Technology, ACS National Meeting, San Francisco, California, September 10-14, 2006.
215. Symposium on Chirality and Enantioselectivity at Surfaces, ACS National Meeting, San Francisco, California, September 10-14, 2006.
216. Symposium on Computational Materials Design in Chemical Industries, ACS National Meeting, San Francisco, California, September 10-14, 2006.
217. Gordon Research Conference on Membranes: Materials and Processes, New London, NH, August 6-11, 2006.
218. Gordon Research Conference on Physical Metallurgy, Plymouth, NH, July 23-26, 2006.
219. Gordon Research Conference on Chemistry at Interfaces, Biddeford, Maine, July 9-14, 2006.
220. Department of Physics, University of Sydney, Sydney, NSW, Australia, May 19, 2006.
221. 135th TMS Annual Meeting, March 12-16, 2006, San Antonio, TX.
222. Center for Low Emission Technologies, University of Queensland, Brisbane Australia, December 2005.
223. ARC Center for Functional Nanomaterials 2nd Annual Meeting, Noosa Heads, Australia, December 2005.
224. Department of Chemical Engineering, University of Melbourne, Melbourne, Australia, November 2005.
225. Center for Molecular Modeling, Swinburne University, Melbourne, Australia, November 2005.
226. China/Japan/USA Joint Chemical Engineering Meeting, Beijing, China, October 11-13, 2005.

227. Department of Chemical Engineering, University of Newcastle, Newcastle, Australia, October 2005.
228. CSIRO Energy Center, Newcastle, Australia, October 2005.
229. ExxonMobil Corporate Research, Annandale, NJ, October 2005.
230. Nanoscale Science and Technology Center, Griffith University, Brisbane, Australia, August 2005.
231. Department of Chemical Engineering and Materials Science, Arizona State University, Tempe, AZ, April 2005.
232. Department of Chemical Engineering, City College of New York, New York, NY, February 2005.
233. Department of Materials Science, University of Pittsburgh, Pittsburgh, PA, February 2005.
234. Department of Chemical Engineering, University of Colorado, Boulder, CO, January 2005.
235. Workshop on Molecular and Particle Processes at Solid Surfaces, San Luis, Argentina, November 2004.
236. ExxonMobil Corporate Research, Annandale, NJ, September 2004.
237. 3rd International Zeolite Membrane Meeting, Breckenridge, CO, July 2004.
238. van't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, Holland, May 2004.
239. Surface Science Center, University of Liverpool, Liverpool, UK, May 2004.
240. Department of Chemistry, University of Cardiff, Cardiff, UK, May 2004.
241. Department of Chemistry, University of Sydney, Sydney, NSW, Australia, May 2004.
242. Department of Physics, University of New England, Armidale, NSW, Australia, May 2004.
243. Department of Chemical Engineering, University of Queensland, Brisbane, Qld., Australia, April 2004.
244. Department of Chemical Engineering, Purdue University, West Lafayette, IN, March 2004.
245. Third San Luis Symposium on Surface Science, Merida, Venezuela, March 2004.
246. Department of Chemistry, Wake Forest University, Winston-Salem, NC, February 2004.
247. Department of Chemistry, Duquesne University, Pittsburgh, PA, January 2004.
248. Surface Analysis session, FACSS 2003 Annual Meeting, Ft. Lauderdale, FL, October 2003.
249. Department of Materials Science and Engineering, University of Florida, Gainesville, FL, October 2003.
250. Department of Chemical Engineering, University of Florida, Gainesville, FL, October 2003.
251. Department of Chemical Engineering, University of Buffalo, Buffalo, NY, October 2003.
252. CECAM Workshop on Simulation of Zeolites: Towards In Silico Design, Lyons, France, October 2003.
253. Department of Physics, Indiana University of Pennsylvania, Indiana, PA, September 2003.

254. Chiral Surfaces Symposium, ACS National Meeting, New Orleans, LA, March 2003.
255. Mechanistic Surface Chemistry Symposium, ACS National Meeting, New Orleans, LA, March 2003
256. Department of Chemical Engineering, University of Missouri at Rolla, January 2003.
257. Pittsburgh-Cleveland Catalysis Society, Pittsburgh, PA, December 2002.
258. Department of Chemical Engineering, University of Wisconsin, December 2002.
259. CAST Plenary Session, AIChE Annual Meeting, Indianapolis, IN, November 2002.
260. Department of Chemical Engineering, University of Delaware, October 2002.
261. Pittsburgh AIChE Chapter, October 2002.
262. Materials Research Seminar, Department of Chemical Engineering, The Pennsylvania State University, October 2002.
263. Chemical Physics/Physical Chemistry Seminar, Departments of Chemistry and Physics, University of Maryland, September 2002
264. GE Corporate Research and Development, Albany, NY, September 2002
265. TDA Inc., Wheatridge, CO, June 2002.
266. National Renewable Energy Laboratory, June 2002.
267. Computational Materials and Biology Group, Sandia National Laboratory, Albuquerque, NM, June 2002.
268. Atomic and Molecular Physics Group, T-Division, Los Alamos National Laboratory, May 2002.
269. Department of Chemical Engineering, University of Massachusetts – Amherst, April 2002.
270. Department of Chemical Engineering, University of Akron, February 2002.
271. Air Products R&D Division, January 2002.
272. Department of Chemical Engineering, University of California at Santa Barbara, Santa Barbara, CA, November 2001.
273. Department of Chemistry, Kent State University, Kent, OH, September 2001.
274. Midwest Thermodynamics and Statistical Mechanics Meeting, East Lansing, MI, May 2001.
275. Computational Materials and Biology Group, Sandia National Laboratory, Albuquerque, NM, December 2000.
276. Department of Chemical Engineering, University of Colorado, October 2000.
277. Department of Applied Mathematics, University of Colorado, October 2000.
278. ExxonMobil Corporate Research Division, Annandale, NJ, June 2000.
279. Air Products and Chemicals Technology Division, Allentown, PA, June 2000.
280. Department of Chemical Engineering, University of Tennessee, April 2000.
281. ACS National Meeting, San Francisco, CA, March 2000 (invited presentation).
282. Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA, October 1999.
283. Condensed Matter Seminar, Department of Physics, Carnegie Mellon University, Pittsburgh, PA, October 1998
284. Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, PA, September 1998

285. Department of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, March 1997.
286. Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA, February 1997.
287. Department of Chemistry, Iowa State University, Ames, IA, January 1997.
288. Department of Applied Mathematics, University of Colorado, Boulder, CO, November 1995.
289. Physics Department, University of New England, Armidale, NSW, Australia, December 1993.
290. 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:

- 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 (Graduated 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. Zhenzi Yu (expected graduation: 5/2022)
48. Yuhan Yang (expected graduation: 5/2022)
49. Alan Daou (expected graduation: 5/2022)
50. Arvind Ganesan [co-advised with Sankar Nair] (expected graduation: 5/2022)
51. Xuqing Cai (expected graduation: 5/2022)
52. Chao-Wen Chang (expected graduation: 5/2023)
53. Ifayoyinsola (Yoyin) Ibikunle (expected graduation: 12/2022)
54. Shubham Jamdade (expected graduation: 5/2023)
55. Xiaohan Yu (expected graduation: 5/2023)
56. Akriti Sarswat [co-advised with Ryan Lively] (expected graduation: 5/2024)
57. Jia Yuan Chng (expected graduation: 5/2024)

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-
20. Dr. Rohan Awati, 9/16-10/18
21. Dr. Alex Hyla, 1/17-12/17
22. Dr. Anh Pham, 1/18-5/18
23. Dr. Farhad Gharagheizi, 6/18-
24. Dr. Raghuram Thyagarajan, 8/18-
25. Dr. Jifeng Sun, 11/18-