

Curriculum Vitae – David S. Sholl

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Education

Ph.D., University of Colorado, Program in Applied Mathematics, Boulder, CO, 1995.
(Advisor: Prof. Rex T. Skodje, Dept. of Chemistry)

M.Sc., University of Colorado, Program in Applied Mathematics, Boulder, CO, 1993.

B.Sc. (with Honors and University Medal), Theoretical Physics,
The Australian National University, Canberra, ACT, Australia, 1992.

Employment

5/25 – present, Executive Director and Vice Provost, University of Tennessee-Oak Ridge
Innovation Institute, Oak Ridge, TN

5/25 – present, Adjunct Professor, School of Chemical & Biomolecular Engineering,
Georgia Institute of Technology, Atlanta, GA

7/23 – 4/24, Interim Executive Director, University of Tennessee-Oak Ridge Innovation
Institute, Oak Ridge, TN

7/21 – present, Director, Transformational Decarbonization Initiative, Oak Ridge
National Laboratory, Oak Ridge, TN

7/21 – 4/24, Professor, School of Chemical & Biomolecular Engineering, Georgia
Institute of Technology, Atlanta, GA

10/16 – 6/21, John F. Brock III School Chair, School of Chemical & Biomolecular
Engineering, Georgia Institute of Technology, Atlanta, GA

7/13 – 9/16, School Chair, School of Chemical & Biomolecular Engineering, Georgia
Institute of Technology, Atlanta, GA

1/08 – 9/16, Michael E. Tennenbaum Family Chair and GRA Eminent Scholar in Energy
Sustainability, School of Chemical and Biomolecular Engineering, Georgia Institute of
Technology, Atlanta, GA

1/10-6/13, Associate Director, Strategic Energy Institute, Georgia Institute of
Technology, Atlanta, GA

7/06-12/07, Professor, Department of Chemical Engineering, Carnegie Mellon
University, Pittsburgh, PA

7/02 – 6/06, Associate Professor, Department of Chemical Engineering, Carnegie Mellon
University, Pittsburgh, PA

8/03 – 12/07, Courtesy Faculty, Department of Materials Science and Engineering,
Carnegie Mellon University, Pittsburgh, PA

1/98 – 6/02, Assistant Professor, Department of Chemical Engineering, Carnegie Mellon
University, Pittsburgh, PA.

2/97-12/97, Postdoctoral researcher, Department of Chemistry, Yale University, New
Haven, CT. (Advisor: Prof. John C. Tully)

2/96-2/97, Postdoctoral researcher, Departments of Chemical Engineering and Physics, The Pennsylvania State University, State College, PA. (Advisor: Prof. Kristen A. Fichthorn)

Leadership Roles

1. Portfolio Strategy Advisor, Department of Energy Office of Clean Energy Demonstrations (OCED), 2022-2023
2. Editor-in-chief, *AIChE Journal*, 2022-present
3. Panel member, National Academies Study Committee, Chemical Engineering: Challenges and Opportunities in the 21st Century, 2020-2021
4. Panel lead, DOE BES Basic Research Needs Workshop on Transformative Manufacturing, 2020
5. Board of Directors, American Institute of Chemical Engineers, 2019-2021
6. Chair, Inaugural Gordon Conference on Chemical Separations, 2020
7. Organizing Committee, Chemical Engineering National Diversity Equity Workshop, 2021
8. Panel member, National Academies Study Committee, Research Agenda for a New Era in Separations Science, 2018-2019
9. Member, AIChE Strategic Plan Steering Committee, 2018
10. Interim Chief Technology Officer (8/16-3/17) and Focus Area Lead (Modeling & Simulation) (3/17-present), RAPID National Manufacturing Institute, AIChE.
11. Co-chair, DOE BES Basic Research Needs Workshop on the Energy-Water Nexus, 2017.
12. School Chair, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, 7/13-6/21.
13. Co-chair, International Conference on Inorganic Membranes 2016.
14. Chair, Gordon Conference on Nanoporous Materials, 8/15.
15. Deputy Director, UNCAGE-ME (DOE Energy Frontier Research Center), 8/14-present.
16. Chair, Computational Molecular Science and Engineering Forum, AIChE, 2012-2014.
17. Co-founder, *InmondoTech Inc.*, 2013-2018
18. Associate Director, Strategic Energy Institute, Georgia Institute of Technology, Atlanta, GA, 1/10-6/13.
19. Senior editor, *Langmuir*, 2009-2019.

Awards and Distinctions

1. Member, US National Academy of Engineering (2024)
2. Georgia Tech Outstanding Achievement in Research Program Development [jointly with several faculty and staff from Georgia Tech] (2024)
3. Kurt Wohl Memorial Lecture, Department of Chemical and Biomolecular Engineering, University of Delaware (2023)
4. Georgia Tech Curriculum Innovation Award [jointly with several faculty from Georgia Tech] (2022)
5. Chemical Engineering Alumni Lectures, University of Massachusetts Amherst (2021)
6. Fellow, American Association for the Advancement of Science (2020)

7. Dumas Lecture in Chemical Engineering, Virginia Tech (2019)
8. Fellow, American Institute of Chemical Engineering (2019)
9. Institute Award for Excellence in Industrial Gases Technology, American Institute of Chemical Engineering (2018)
10. Parr Lecturer, Department of Chemical and Biomolecular Engineering, University of Illinois (2018)
11. "Highly Prolific Author" recognition, Journal of Physical Chemistry C (2017)
12. AIChE Gary Leach Award [jointly with several faculty and staff from Georgia Tech] (2015)
13. Early Career Achievement Award, Computational Molecular Science and Engineering Forum, AIChE (2010)
14. DOE Hydrogen Program R&D Award (2008)
15. MESD Plenary Session speaker, AIChE Annual Meeting (2007)
16. COMSEF Plenary Session speaker, AIChE Annual Meeting (2006)
17. CAST Plenary Session speaker, AIChE Annual Meeting (2002)
18. Camille Dreyfus Teacher-Scholar Award (2002)
19. E. Kears Pollock/PPG Industries Grant for Young Faculty (2002-2005)
20. Alfred P. Sloan fellow (2001-2003)
21. George Tallman Ladd Award for Excellence in Research, Carnegie Institute of Technology, Carnegie Mellon University (2000)
22. National Science Foundation CAREER Award (2000-2004)
23. Faculty Fellow, National Energy Technology Laboratory (2000-2007)
24. APS Division of Chemical Physics Travel Award (1996).
25. University of Colorado Graduate School Research and Creative Work Award (1995).
26. Honorable mention, NSF Graduate Research Fellowship (1991).
27. University of Colorado Doctoral Fellowship (1991).
28. University Medal, Australian National University (1991).
29. Education Abroad Scholar, University of California (1988-1989).
30. National Undergraduate Scholarship, Australian National University (1987-1991).

Research Publications (> 28,000 citations, h-index = 88 as reported by Web of Science; > 39,000 citations, h-index = 101 as reported by Google Scholar)
 [Publications with > 50 citations in Web of Science indicated by * and with > 100 citations indicated by **]

1. *Machine learning and IAST-aided high-throughput screening of cationic and silica zeolites for alkane capture, storage, and separations*, Alan S. S. Daou, Hanjun Fang, Salah Eddine Boulfefel, Peter I. Ravikovitch, and David S. Sholl, Journal of Physical Chemistry C, 128 (2024), 6089-6105
2. *Probing structural defects in MOFs using water stability*, Shubham Jamdade, Zhenzi Yu, Salah Eddine Boulfefel, Xuqing Cai, Raghuram Thyagarajan, Hanjun Fang, and David S. Sholl, Journal of Physical Chemistry C, 128 (2024) 3975-3984
3. *Discovering dinuclear dioxygen-bridged cobalt(III) complexes for selective binding of O₂ from air*, Jifeng Sun, Hanjun Fang, Farhad Gharagheizi, Peter I. Ravikovitch, and David S. Sholl, Journal of Physical Chemistry C, 128 (2023) 474-482

4. *Machine learning models for predicting molecular diffusion in metal-organic frameworks accounting for the impact of framework flexibility*, Yuhan Yang, Zhenzi Yu, and David S. Sholl, *Chemistry of Materials*, 35 (2023) 10156-10168
5. *Computational screening of cationic zeolites for n-butane/methane separations using quantitatively accurate first-principles-derived force fields*, Hanjun Fang, Alan S. S. Daou, Salah Eddine Boulfelfel, John M. Findley, Peter I. Ravikovitch, and David S. Sholl, *Journal of Physical Chemistry C*, 127 (2023) 23941-23955
6. *Structural and adsorption properties of ZIF-8-7 hybrid materials synthesized by acid gas-assisted and de novo routes*, Arvind Ganesan, Peter C. Metz, Raghuram Thyagarajan, Yuchen Chang, Stephen C. Purdy, Krishna C. Jayachandrababu, Katharine Page, David S. Sholl, and Sankar Nair, *Journal of Physical Chemistry C*, 127 (2023) 23956-23965
7. *Does mixed linker-induced heterogeneity impact the accuracy of IAST predictions in UiO-66-NH₂?*, Lukas W. Bingel, Zhenzi Yu, David S. Sholl, and Krista S. Walton, *Journal of Physical Chemistry C*, 127 (2023) 20881-20889
8. *Quantum chemical simulations of CO₂ and N₂ capture in reline, a prototypical deep eutectic solvent*, Jacek Jakowski, Jingsong Huang, Syed Z. Islam, and David S. Sholl, *Journal of Physical Chemistry B*, 127 (2023) 8888-8899
9. *Hierarchical ZIF-8 materials via acid gas-induced defect sites: synthesis, characterization, and functional properties*, Arvind Ganesan, Johannes Leisen, Raghuram Thyagarajan, David S. Sholl, and Sankar Nair, *ACS Applied Materials & Interfaces*, 15 (2023) 40623-40632
10. *An effective air-liquid contactor for CO₂ direct air capture using aqueous solvents*, Abishek Kasturi, Gyoung Gug Jang, Adeola Dona-Tella Akin, Amiee Jackson, Jiheon Jun, Diana Stamberg, Radu Custelcean, David S. Sholl, Sotira Yiaccoumi, and Costas Tsouris, *Separation and Purification Technology*, 324 (2023) 124398
11. *Efficient exploration of adsorption space for separations in metal-organic frameworks combining the use of molecular simulations, machine learning, and Ideal Adsorbed Solution Theory*, Xiaohan Yu, Dai Tang, Jia Yuan Chng, and David S. Sholl, *Journal of Physical Chemistry C*, 127 (2023) 19229-19239
12. *Quantitative simulations of siloxane adsorption in metal-organic frameworks*, Jia Yuan Chng and David S. Sholl, *ACS Applied Materials & Interfaces*, 15 (2023) 37828-37836
13. *Efficient generation of large collections of metal-organic framework structures containing well-defined point defects*, Zhenzi Yu, Shubham Jamdade, Xiaohan Yu, Xuqing Cai, and David S. Sholl, *Journal of Physical Chemistry Letters*, 14 (2023) 6658-6665
14. *Selective uptake of ethane/ethylene mixtures by UTSA-280 is driven by reversibly coordinated water defects*, Yutao Gong, Xuqing Cai, Wenqin You, Xiao Jiang, Wei Liu, Ryan Lively, Krista S. Walton, and David S. Sholl, *Chemistry of Materials*, 35 (2023) 2956-2966
15. *A membrane contactor enabling energy-efficient CO₂ capture from point sources with deep eutectic solvents*, Syed Z. Islam, Md Arifuzzaman, Gernot Rother, Vera Bocharova, Robert L. Sacci, Jacek Jakowski, Jingsong Huang, Ilia Nicolaevich Ivanov, Ramesh R. Bhave, Tomonori Saito, and David S. Sholl, *Industrial & Engineering Chemistry Research*, 62 (2023) 4455-4465

16. *Strong degradation of polycarbonate and polystyrene by the CO₂ capture solvent diethyl sebacate*, Syed Z. Islam, David S. Sholl, Janice A. Steckel, and Robert L. Thompson, *Process Safety Progress*, 42 (2023) 371-376
17. *New data sharing requirements for AIChE Journal authors*, David S. Sholl, *AIChE Journal*, 69 (2023) e18017
18. *Identifying high-performance metal-organic frameworks for low-temperature oxygen recovery from helium by computational screening*, Shubham Jamdade, Rishi Gurnani, Hanjun Fang, Salah Eddine Boulfefel, Rampi Ramprasad, and David S. Sholl, *Industrial & Engineering Chemistry Research*, 62 (2023) 1927-1935
19. *Development of porous crystalline materials for selective binding of O₂ from air*, Jifeng Sun, Farhad Gharagheizi, Hanjun Fang, Peter I. Ravikovitch, and David S. Sholl, *Journal of Physical Chemistry C*, 127 (2023) 776-787
20. *Assessment of Acid Gas Adsorption Selectivities in MIL-125-NH₂*, Chunyi Li, Zhenzhi Yu, Kai Cui, J. R. Schmidt, David S. Sholl, and Ryan P. Lively, *Journal of Physical Chemistry C*, 126 (2022) 21414-21425
21. *Adapting UFF4MOF for heterometallic rare-earth metal-organic frameworks*, Yuhan Yang, Ifayoyinsola A. Ibikunle, Dorina F. Sava Gallis, and David S. Sholl, *ACS Applied Materials & Interfaces*, 14 (2022) 54101-54110
22. *Trends in siting of metals in heterometallic Nd-Yb metal-organic frameworks and molecular crystals*, Ifayoyinsola A. Ibikunle, Yuhan Yang, Nichole R. Valdez, Mark A. Rodriguez, Jacob A. Harvey, Dorina F. Sava Gallis, and David S. Sholl, *ACS Applied Materials & Interfaces*, 14 (2022) 54349-54358
23. *Assessment of acid gas adsorption selectivities in MIL-125-NH₂*, Chunyi Li, Zhenzi Yu, Kai Cui, J. R. Schmidt, David S. Sholl and Ryan P. Lively, *Journal of Physical Chemistry C*, 126 (2022) 21414-21425
24. *Theoretical pathway towards improved reverse osmosis membrane selectivity for neutral solutes: Inspiration from gas separations*, Haley D. White, Hannah G. Huang, Margaret C. D'Amaro, Elisa A. Mignone, David S. Sholl, and Ryan P. Lively, *Journal of Physical Chemistry C*, 126 (2022) 19496-19506
25. *Unlocking a rigid purine MOF for kinetic separation of xylenes*, Richelle Lyndon, Yuxiang Wang, Ian M. Walton, Yao Ma, Yang Liu, Zhenzi Yu, Guanghui Zhu, Samuel Berens, Yu-Sheng Chen, SuYin Wang, Sergey Vasenkov, David S. Sholl, Krista S. Walton, Simon H. Pang, and Ryan P. Lively, *Chemical Communications*, 58 (2022) 12305-12308
26. *Achieving order of magnitude increases in CO₂ reduction reaction efficiency by product separations and recycling*, Akriti Sarswat, David S. Sholl, and Ryan P. Lively, *Sustainable Energy & Fuels*, 6 (2022) 4598-4604
27. *Online graduate certificate in data science for the chemical industry*, Andrew Medford, Fani Boukouvala, Martha Grover, David Sholl, Carson Meredith, Pengfei Cheng, Sihoon Choi, Gabriel Gusmao, Zachary Kilwein, Suryateja Ravutla, Fatimah Wirth, Zaid Sewer, Jennifer Wooley, *Chemical Engineering Education*, 56 (2022) 249-259
28. *Metal-organic Framework Integrating Framework and Bimetallic Coupling Effect for Highly Efficient Oxygen Evolution Reaction*, Shulin Li, Tienan Wang, Dai Tang, Yuting Yang, Yuyang Tian, Fengchao Cui, Jifeng Sun, Xiaofei Jing, David S. Sholl, and Guangshan Zhu, *Advanced Science*, 9 (2022) 2203712

29. *Curated Collection of More than 20,000 Experimentally-reported One-Dimensional Metal-Organic Frameworks*, Farhad Gharagheizi, Zhenzi Yu, and David S. Sholl, ACS Applied Materials & Interfaces, 14 (2022) 42258-42266
30. *Point defects control guest diffusion in the 1D pores of Zn(tbip)*, Xuqing Cai and David S. Sholl, Journal of Physical Chemistry C, 126 (2022) 14321-14328
31. *Kinetic model of acid gas induced defect propagation in zeolitic imidazolate frameworks*, Kai Cui, Sankar Nair, David S. Sholl, and J. R. Schmidt, Journal of Physical Chemistry Letters, 13 (2022) 6541-6548
32. *Experimentally verified alkane adsorption isotherms in nanoporous materials from literature meta-analysis*, Lukas W. Bingel, Krista S. Walton, and David S. Sholl, Journal of Chemical and Engineering Data, 67 (2022) 1757-1764
33. *Discrepancy quantification between experimental and simulated data of CO₂ adsorption isotherm using hierarchical Bayesian estimation*, Sotaro Kojima, Jongwoo Park, Eli A. Carter, Krista S. Walton, Matthew J. Realff, David S. Sholl, Tomoyuki Yajima, Junpei Fujiki and Yoshiaki Kawajiri, Separation and Purification Technology, 296 (2022) 121371
34. ***How reproducible are surface areas calculated from the BET equation?* Johannes W. M. Osterrieth, Jarnes Rampersad, David Madden, David S. Sholl, David Fairen-Jiminez et al. [>50 authors in total], Advanced Materials, 34 (2022) 2201502
35. *Gaussian approximation of dispersion potentials for efficient featurization and machine-learning predictions of metal-organic frameworks*, Sihoon Choi, David S. Sholl, and Andrew J. Medford, Journal of Chemical Physics, 156 (2022) 214108
36. *Effect of loading on the water stability of the metal-organic framework DMOF [Zn(bdc)(dabco)_{0.5}]*, Carmen Chen, Zhenzi Yu, David S. Sholl and Krista S. Walton, Journal of Physical Chemistry Letters, 13 (2022) 4891-4896
37. *Molecular simulations of CH₄ and CO₂ diffusion in rigid amorphous materials*, Raghu Thyagarajan and David S. Sholl, Journal of Physical Chemistry C, 126 (2022) 8530-8538
38. *In silico design of microporous polymers for chemical separations and storage*, Dylan M. Anstine, David S. Sholl, Joern Ilja Siepmann, Randall Q. Snurr, Alán Aspuru-Guzik and Coray M. Colina, Current Opinion in Chemical Engineering, 36 (2022) 100795
39. *Accelerating solvent selection for type II porous liquids*, Chao-Wen Chang, Isaiah Borne, Robin M. Lawler, Zhenzhi Yu, Seung Soon Jang, Ryan P. Lively and David S. Sholl, Journal of the American Chemical Society, 144 (2022) 4071-4079
40. *A systematic examination of the impacts of MOF flexibility on intracrystalline molecules diffusivities*, Yuhan Yang and David S. Sholl, Journal of Materials Chemistry A, 10 (2022) 4242-4253
41. *Exemplar mixtures for studying complex mixture effects in practical chemical separations*, David S. Sholl and Ryan P. Lively, JACS Au, 2 (2022) 322-327
42. *Opening the toolbox: 18 experimental techniques for measurements of mixed gas adsorption*, Danny Shade, Brandon W. S. Bout, David S. Sholl and Krista S. Walton, Industrial & Engineering Chemistry Research 61 (2022) 2367-2391
43. *Single-walled zeolitic nanotubes*, Akshay Korde, Byunghyun Min, Elina Kapaca, Omar Knio, Iman Nezam, Ziyuan Wang, Johannes Leisen, Xinyang Yin, Xueyi

- Zhang, David S. Sholl, Xiaodong Zou, Tom Wilhammar, Christopher W. Jones and Sankar Nair, *Science*, 375 (2022) 62
44. *Comprehensive assessment of the accuracy of the Ideal Adsorbed Solution Theory for predicting binary adsorption of gas mixtures in porous materials*, Farhad Gharagheizi and David S. Sholl, *Industrial & Engineering Chemistry Research*, 61 (2022) 727-739
 45. *Incorporating flexibility effects into metal-organic framework adsorption simulations using different models*, Zhenzi Yu, Dylan M. Anstine, Salah Eddine Boulfefel, Chenkai Gu, Coray M. Colina and David S. Sholl, *ACS Applied Materials & Interfaces*, 13 (2021) 61305-61315
 46. *A transferable force field for predicting adsorption and diffusion of small molecules in alkali exchanged zeolites with coupled cluster accuracy*, Salah Eddine Boulfefel, John M. Findley, Hanjun Fang, Alan S. S. Daou, Peter I. Ravikovitch and David S. Sholl, *Journal of Physical Chemistry C*, 125 (2021) 26832-26846
 47. *Computational screening of MOFs and zeolites for direct air capture of carbon dioxide under humid conditions*, John M. Findley and David S. Sholl, *Journal of Physical Chemistry C*, 125 (2021) 24630-24639
 48. *Controlled demolition and reconstruction of imidazolate and carboxylate metal-organic frameworks by acid gas exposure and linker treatment*, Arvind Ganesan, Stephen C. Purdy, Zhenzi Yu, Souryadeep Bhattacharyya, Katharine Page, David S. Sholl and Sankar Nair, *Industrial & Engineering Chemistry Research*, 60 (2021) 15582-15592
 49. **High throughput screening of anion-pillared metal-organic frameworks for the separation of light hydrocarbons*, Chenkai Gu, Jing Liu and David S. Sholl, *Journal of Physical Chemistry C*, 125 (2021) 20076-20086
 50. *Analysis of energetics and economics of sub-ambient hybrid post-combustion carbon dioxide capture*, Stephen J. A. DeWitt, Rohan Awati, Hector Octavio Rubiera Landa, Jongwoo Park, Yoshiaki Kawajiri, David S. Sholl, Matthew J. Realff and Ryan P. Lively, *AIChE Journal* (2021) e17403
 51. *Efficient models for predicting temperature-dependent Henry's constants and adsorption selectivities for diverse collections of molecules in metal-organic frameworks*, Xiaohan Yu, Sihoon Choi, Dai Tang, Andrew J. Medford and David S. Sholl, *Journal of Physical Chemistry C*, 125 (2021) 18046-18057
 52. *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
 53. *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
 54. *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 Boulfefel, Hanjun Fang, Giovanni Muraro, Peter I. Ravikovitch and David S. Sholl, *Journal of Physical Chemistry C* 125 (2021) 8418-8429

55. *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
56. *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
57. *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
58. *Adsorption-based separation of near-azeotropic mixtures: a challenging example for high-throughput development of adsorbents*, Dai Tang, Farhad Gharagheizi and David S. Sholl, Journal of Physical Chemistry B 125 (2021) 926
59. *A collection of more than 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
60. *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
61. *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/jpc.0c08629
62. *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, Ivo Hermans, David S. Sholl and Carsten Sievers, ChemCatChem, DOI: 10.1002/cctc.202001424
63. *A database of porous rigid amorphous materials*, Raghuram Thyagarajan and David S. Sholl, Chemistry of Materials, 32 (2020) 8020-8033
64. *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
65. *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
66. *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
67. *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

68. *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
69. *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
70. *How well do approximate models of adsorption-based CO₂ 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
71. *Impact of intrinsic framework flexibility for selective adsorption of sarin in non-aqueous solvents using metal-organic frameworks*, Jongwoo Park, Mayank Agrawal, Dorina F. Sava Gallis, Jacob A. Harvey, Jeffrey A. Greathouse, and David S. Sholl, Physical Chemistry Chemical Physics, 22 (2020) 6441-6448
72. *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
73. *Watching Water, Sodium, and Chloride Passing through a Graphitic Pore*, David S. Sholl, Matter, 2 (2020) 524-525
74. *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
75. *A strong test of atomically detailed model of molecular adsorption in zeolites using multilaboratory experimental data for CO₂ 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
76. *Does repeat synthesis in materials chemistry obey a power law?* Mayank Agrawal, Rebecca Han, Dinushka Herath and David S. Sholl, Proceedings of the National Academies of Science, 117 (2020) 877-822
77. *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
78. *Quantitative correlations for the durability of zeolitic imidazolate frameworks in humid SO₂*, Souryadeep Bhattacharyya, David S. Sholl and Sankar Nair, Industrial and Engineering Chemistry Research, 59 (2020) 245-252
79. *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
80. ****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
81. *Five easy ways to make your research more reproducible*, David S. Sholl, *Langmuir*, 35 (2019) 13257-13258
 82. *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
 83. *In-situ ATR-IR study of surface reaction during aqueous phase reforming of glycerol, sorbitol and glucose over Pt/ γ -Al₂O₃*, Jungseob So, Yoona Chung, David S. Sholl, and Carsten Sievers, *Molecular Catalysis*, 475 (2019) 110423
 84. **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
 85. *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 Boulfefel, Giovanni Muraro, Charanjit Paur, Karl Strohmaier, Peter I. Ravikovitch and David S. Sholl, *Journal of Physical Chemistry C*, 123 (2019) 20405-20412
 86. *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
 87. *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
 88. *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
 89. *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
 90. *Predictions of Hg⁰ and HgCl₂ adsorption properties in UiO-66 from flue gas using molecular simulations*, Hongjian Tang, Hanjun Fang, Yufeng Duan and David S. Sholl, *Journal of Physical Chemistry C*, 123 (2019) 5972-5979
 91. *Screening diffusion of small molecules in flexible zeolitic imidazolate frameworks using a DFT parameterized force field*, Ross J. Verploegh, Ambarish Kulkarni, Salah Eddine Boulfefel, Jonathan C. Haydak, Dai Tang and David S. Sholl, *Journal of Physical Chemistry C*, 123 (2019) 9153-9167
 92. *Stability of zeolitic imidazolate frameworks in NO₂*, Souryadeep 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
 93. *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

94. *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
95. *Moving beyond adsorption capacity in design of adsorbents for CO₂ capture from ultradilute feeds: Kinetics of CO₂ adsorption in materials with stepped isotherms*, Lalit A. Darunte, Trisha Sen, Chiraag Bhawanani, Krista S. Walton, David S. Sholl, Matthew J. Realff, and Christopher W. Jones, *Industrial & Engineering Chemistry Research*, 58 (2019) 366-377
96. *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
97. **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
98. *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
99. *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
100. **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
101. *First-principles-derived force fields for CH₄ adsorption and diffusion in siliceous zeolites*, Hanjun Fang, Rohan Awati, Salah E. Boulfefel, Peter I Ravikovitch, and David S. Sholl, *Journal of Physical Chemistry C*, 122 (2018) 12880-12891
102. *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
103. *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
104. *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
105. *Quantitative predictions of molecular diffusion in binary mixed-linker zeolitic imidazolate frameworks using molecular simulation*, Ross J. Verploegh, Ying Wu, Salah Eddine Boulfefel and David S. Sholl, *Journal of Physical Chemistry C*, 122 (2018) 5627-5638
106. **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

107. *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
108. *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
109. *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
110. ***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
111. **CO₂ dynamics in pure and mixed-metal MOFs with open metal sites*, Robert M. Marti, Joshua D. Howe, Cody R. Morelock, Mark S. Conradi, Krista S. Walton, David S. Sholl and Sophia E. Hayes, *Journal of Physical Chemistry C*, 121 (2017) 25778-25787
112. *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
113. *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
114. *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
115. *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
116. **Effect of surface structure of TiO₂ nanoparticles on CO₂ adsorption and SO₂ resistance*, Uma Tumuluri, Joshua D. Howe, William P. Mounfield, Meijun Li, Miaofang Chi, Zachary D. Hood, Krista S. Walton, David S. Sholl, Sheng Dai and Zili Wu, *ACS Sustainable Chemistry & Engineering*, 5 (2017) 9295-9306
117. *Butanol separation from humid CO₂-containing multicomponent vapor mixtures by zeolitic imidazolate frameworks*, Souryadeep Bhattacharyya, Krishna C. Jayachandrababu, Yadong Chiang, David S. Sholl and Sankar Nair, *ACS Sustainable Chemistry & Engineering*, 5 (2017) 9467-9476
118. *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

119. **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
120. *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
121. *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
122. *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
123. *First-principles investigation of chemical stability and proton conductivity in M-doped BaZrO₃ (M = K, Rb, and Cs)*, *Journal of the American Ceramic Society*, 100 (2017) 2997-3003
124. *Establishing upper bounds on CO₂ swing capacity in sub-ambient pressure swing adsorption via molecular simulation of metal-organic frameworks*, Jongwoo Park, Ryan P. Lively and David S. Sholl, *Journal of Materials Chemistry A*, 5 (2017) 12258-12265
125. **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
126. **Monolith-supported amine-functionalized Mg₂(dobpdc) adsorbents for CO₂ capture*, Lalit A. Darunte, Yuri Terada, Christopher R. Murdock, Krista S. Walton, David S. Sholl, and Christopher W. Jones, *ACS Applied Materials and Interfaces*, 9 (2017) 17043-17051
127. ***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
128. *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
129. ***From water to organics in membrane separations*, Ryan P. Lively and David S. Sholl, *Nature Materials* 16 (2017) 276-279
130. **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
131. **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

132. *Computational investigation on CO₂ adsorption in titanium carbide-derived carbons with residual titanium*, Difan Zhang, Michael R. Dutzer, Tao Liang, Alexandre F. Fonseca, Ying Wu, Krista S. Walton, David S. Sholl, Amir H. Farmahini, Suresh K. Sinnott, and Susan B. Sinnott, *Carbon*, 111 (2017) 741-751
133. *Characterizing chemical stability and proton conductivity of B-site doped barium hafnate (BaHfO₃) and barium stannate (BaSnO₃) with first principles modeling*, Sung Gu Kang and David S. Sholl, *Journal of Alloys and Compounds*, 693 (2017) 738-743
134. ***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
135. *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
136. ***Interactions of SO₂-containing acid gases with ZIF-8: Structural changes and mechanistic investigations*, Souryadeep Bhattacharyya, Simon H. Pang, Michael R. Dutzer, Ryan P. Lively, Krista S. Walton, David S. Sholl and Sankar Nair, *Journal of Physical Chemistry C*, 120 (2016) 27221-27229
137. **Synergistic effects of water and SO₂ on degradation of MIL-125 in the presence of acid gases*, William P. Mounfield III, Chu Han, Simon H. Pang, Uma Tumuluri, Yang Jiao, Souryadeep Bhattacharyya, Michael R. Dutzer, Sankar Nair, Zili Wu, David S. Sholl and Krista S. Walton, *Journal of Physical Chemistry C*, 120 (2016) 27230-27240
138. **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
139. ***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
140. *One-Step Synthesis of Zeolite Membranes Containing Catalytic Metal Clusters*, Seok-Jhin Kim, Shuai Tan, Micaela Taborga Claire, Laura Gil Briones, Karren L. More, Yujun Liu, Jason S. Moore, Ravindra S. Dixit, John G. Pendergast, David S. Sholl, Christopher W. Jones and Sankar Nair, *ACS Applied Materials and Interfaces*, 37 (2016) 24671-24681
141. **Propane dehydrogenation over alumina-supported iron/phosphorous catalysts: Structural evolution of iron species leading to high activity and propylene selectivity*, Shuai Tan, Bo Hu, Wun-Gwi Kim, Simon H. Pang, Jason S. Moore, Yujun Liu, Ravindra S. Dixit, John G. Pendergast, David S. Sholl, Sankar Nair, Christopher W. Jones, *ACS Catalysis*, 6 (2016) 5673-5683
142. *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
143. *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

144. ****CO₂ via adsorption in amine-functionalized sorbents**, Lalit A. Darunte, Krista S. Walton, David S. Sholl and Christopher W. Jones, *Current Opinion in Chemical Engineering*, 12 (2016) 82-90
145. *Structure elucidation of mixed-linker zeolitic imidazolate frameworks by solid-state H¹CRAMPS 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
146. *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
147. ***Identification of high-CO₂-capacity cationic zeolites by accurate computational screening**, Hanjun Fang, Ambarish Kulkarni, Preeti Kamakoti, Rohan Awati, Peter I. Ravikovitch, and David S. Sholl, *Chemistry of Materials*, 28 (2016) 3887-3896
148. *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
149. ****Direct air capture of CO₂ 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
150. *Effects of Open Metal Site Availability on Adsorption Capacity and Olefin/Paraffin Selectivity in the Metal-Organic Framework Cu₃(BTC)₂*, Jason Bentley, Guo Shiou Foo, Meha Rungta, Sangar Neeraj, Carsten Sievers, David S. Sholl, and Sankar Nair, *Industrial and Engineering Chemistry Research*, 55 (2016) 5043-5053
151. ****Seven Chemical Separations To Change The World**, David S. Sholl and Ryan P. Lively, *Nature*, 532 (2016), 435-437
152. ****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
153. *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
154. *Effect of framework flexibility on C₈ aromatic adsorption at high loadings in metal-organic frameworks*, Jason A. Gee and David S. Sholl, *Journal of Physical Chemistry C*, 120 (2016) 370-376
155. ****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
156. ****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

157. *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
158. **High T_c layered ferrielectric crystals by coherent spinodal decomposition*, Michael A. Susner, Alex Belianinov, Albina Borisevich, Qian He, Marius Chyasnovich, Hakan Demir, David S. Sholl, Panchapakesan Ganesh, Douglas L. Abernathy, Michael A. McGuire and Petro Maksymovch, *ACS Nano*, 9 (2015) 12365-12373
159. *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
160. *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
161. **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
162. **Defects in metal-organic frameworks: Challenge or opportunity?*, David S. Sholl and Ryan P. Lively, *Journal of Physical Chemistry Letters*, 6 (2015) 3437-3444
163. *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
164. ***Predicting multicomponent adsorption: 50 years of the ideal adsorbed solution theory*, Krista S. Walton and David S. Sholl, *AIChE Journal*, 61 (2015) 2757-2762
165. *DFT-derived force fields for modeling hydrocarbon adsorption in MIL-47(V)*, Ambarish R. Kulkarni and David S. Sholl, *Langmuir*, 31 (2015) 8453-8468
166. *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
167. *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
168. *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
169. **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
170. *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
171. *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
172. *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
173. *Selection of surface coatings for high H₂ permeability group 5 metal membranes using first-principles calculations*, Rongshun Zhu, Shiqiang Hao, and David S. Sholl, *J. Phys. Chem. C* 119 (2015) 7848-7855
174. ***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
175. *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
176. *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
177. ***The materials genome in action: identifying the performance limits for methane storage*, Cory M. Simon, Jihan Kim, Diego A. Gomez-Gualdrón, 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
178. *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
179. *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
180. **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
181. *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
182. *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

183. *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
184. *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
185. *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
186. *Investigating energetics of Au₈ 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
187. *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
188. ***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
189. ***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
190. *First-principles study of chemical stability of the lithium oxide garnets Li₇La₃M₂O₁₂ (M = Zr, Sn, or Hf)*, S. G. Kang and D. S. Sholl, *J. Phys. Chem. C*, 118 (2014) 17402-17406
191. **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
192. *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
193. *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
194. *First principles studies of proton conduction in KTaO₃*, Sung Gu Kang and David S. Sholl, *J. Chem. Phys.*, 141 (2014) 024707
195. ***Thermal, oxidative and CO₂ induced degradation of primary amines used for CO₂ 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
196. *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
197. *Quantitative computational screening of Pd-based intermetallic membranes for hydrogen separation*, Nita Chandrasekhar and David S. Sholl, *J. Membrane Science*, 453 (2014) 516-524

198. *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
199. ***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
200. *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
201. *Predicting low pressure O₂ 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
202. ***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
203. **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
204. *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
205. *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
206. *Near surface phase transition of solute derived Pt monolayers*, Robert E. Rettew, Shuang Cheng, Marc Sauerbrey, Thomas A. Manz, David S. Sholl, Chernoy Jaye, Daniel A. Fischer, and Faisal M. Alamgir, *Topics in Catalysis*, 56 (2013) 1065-1073
207. **Efficient and accurate methods for characterizing effects of framework flexibility on molecular diffusion in zeolites: CH₄ 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
208. **MOF stability and gas adsorption as a function of exposure to water, humid air, SO₂, and NO₂*, 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
209. *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
210. **Surface interactions of C₂ and C₃ polyols with γ -Al₂O₃ and the role of coadsorbed water*, John R. Copeland, Xue-Rong Shi, David S. Sholl, and Carsten Sievers, *Langmuir* 29 (2013) 581-593
211. **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

212. *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
213. ***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
214. *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
215. *First principles models of facilitating H₂ transport through metal films using spillover*, Shiqiang Hao and David S. Sholl, *J. Phys. Chem. C*, 117 (2013) 1217-1223
216. *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
217. ***Rational tuning of water vapor and CO₂ 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
218. *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
219. *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
220. *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
221. *Quantifying large effects of framework flexibility on diffusion in MOFs: CH₄ and CO₂ in ZIF-8*, Emmanuel Haldoupis, Taku Watanabe, Sankar Nair, and David S. Sholl, *ChemPhysChem*, 13 (2012) 3449-3452
222. ***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)
223. ***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
224. ***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
225. ***Analysis of equilibrium-based TSA processes for direct capture of CO₂ from air*, Ambarish Kulkarni and David S. Sholl, *Ind. Eng. Chem. Res.* 51 (2012) 8631-8645
226. ***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
227. ****Prediction of CO₂ 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
228. *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
229. *Nucleation of Rh_n (n = 1-5) clusters on α-Al₂O₃ surfaces: Density functional theory study*, Xue-Rong Shi and David S. Sholl, *J. Phys. Chem. C*, 116 (2012) 10623-10631
230. ****Role of amine structure on CO₂ 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
231. *Antiphase domain boundaries at the Fe₃O₄(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
232. ****Modification of the Mg/DOBDC MOF with Amines to Enhance CO₂ 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
233. ****Ultem/ZIF-8 Mixed Matrix Hollow Fiber Membranes for CO₂/N₂ Separations**, Ying Dai, J. R. Johnson, Oguz Karvan, David S. Sholl, and W. J. Koros, *J. Membrane Science*, 401-402 (2012) 76-82
234. ***High-Throughput Screening of MOFs for CO₂ 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
235. ****Finding MOFs for Highly Selective CO₂/N₂ 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
236. ***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
237. *Predictions of sulfur resistance in metal membranes for H₂ purification using first-principles calculations*, Ki Chul Kim, Sung Gu Kang and David S. Sholl, *Ind. Eng. Chem. Res.*, 51 (2012) 301-309
238. ***Effect of TiH₂-induced strain on thermodynamics of hydrogen release from MgH₂**, Shiqiang Hao and David S. Sholl, *J. Phys. Chem. C*, 116 (2012) 2045-2050
239. *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

240. **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
241. *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
242. *Preparation and Gas Adsorption Characteristics of Zeolite MFI Crystals with Organic-Modified Interiors*, Mohamad H. Kassae, David S. Sholl and Sankar Nair, *J. Phys. Chem. C*, **115** (2011) 19640-19646
243. *New fundamental experimental studies on α -Mg(BH₄)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
244. *Computational prediction of durable amorphous metal membranes for H₂ purification*, Shiqiang Hao and David S. Sholl, *Journal of Membrane Science*, **381** (2011) 192-196
245. *Sonochemical synthesis and characterization of sub-micron crystals of the metal-organic framework Cu[(hfiipbb)(H₂hfiipbb)_{0.5}]*, Cantwell G. Carson, Andrew J. Brown, David S. Sholl, and Sankar Nair, *Crystal Growth and Design*, **11** (2011) 4505-4510
246. *A porous maze*, David S. Sholl, *Nature Chemistry* **3** (2011) 429-430 [research highlight]
247. **Molecular simulations and theoretical predictions for adsorption and diffusion of CH₄/H₂ and CO₂/CH₄ mixtures in ZIFs*, Jinchen Liu, Seda Keskin, David S. Sholl, and J. Karl Johnson, *J. Phys. Chem. C* **115** (2011) 12560-12566
248. *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
249. *Chemical speciation of adsorbed glycine on metal surfaces*, Jeong Woo Han and David S. Sholl, *J. Chem. Phys.* **135** (2011) 034703
250. *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.
251. *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
252. **Pore size analysis of > 250,000 hypothetical zeolites*, Emmanuel Haldoupis, Sankar Nair, and David Sholl, *Physical Chemistry Chemical Physics*, **13** (2011) 5053-5060.
253. *First principles screening of PdCuAg ternary alloys as H₂ purification membranes*, Chen Ling, Lymarie Semidey-Flecha, and David S. Sholl, *J. Membrane Science*, **371** (2011) 189-196

254. *Surface reactions of AsH₃, H₂Se, and H₂S on the Zn₂TiO₄(010) surface*, Shiqiang Hao, Rees B. Rankin, J. Karl Johnson, and David S. Sholl, *Surface Science*, **605** (2011) 818-823
255. *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
256. **Density functional theory study of H and CO adsorption on alkali-promoted Mo₂C surfaces*, Jeong Woo Han, Liwei Li, and David S. Sholl, *J. Physical Chemistry C*, **115** (2011) 6870-6876
257. **AZn₂(BH₄)₅ (A = Li, Na) and NaZn(BH₄)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
258. *Role of Schottky defects in hydrogen and metal diffusion in NaH, MgH₂, and NaMgH₃*, Shiqiang Hao and David S. Sholl, *J. Physical Chemistry Letters*, **1** (2010) 2968-2973
259. *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
260. *First-principles characterization of amorphous phases of MB₁₂H₁₂, 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
261. *Enantiospecific adsorption of amino acids on hydroxylated quartz (10-10)*, Jeong Woo Han and David S. Sholl, *Physical Chemistry Chemical Physics*, **12** (2010) 8024-8032
262. *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
263. ***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.
264. ***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.
265. *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.
266. **Molecular chemisorption on open metal sites in Cu₃(BTC)₂: A spatially periodic density functional theory study*, Taku Watanabe and David S. Sholl, *J. Chem. Phys.* **133** (2010) 094509
267. ***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.

268. *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
269. *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
270. ***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
271. *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
272. *The role of interstitial H₂ in hydrogen diffusion in light metal borohydrides*, Shiqiang Hao and David S. Sholl, *Phys. Chem. Chem. Phys.*, **11** (2009) 11106-11109.
273. **Crystal structures and thermodynamic investigations of LiK(BH₄)₂, KBH₄, and NaBH₄ from first-principles calculations*, Ki Chul Kim and David S. Sholl, *J. Phys. Chem. C*, **114** (2010) 678-686
274. **Computational Identification of a Metal Organic Framework for High Selectivity Membrane-based CO₂/CH₄ Separations: Cu(hfipbb)(H₂hfipbb)_{0.5}*, Taku Watanabe, Seda Keskin, Sankar Nair, and David S. Sholl, *Phys. Chem. Chem. Phys.*, **11** (2009) 11389-11394
275. *First principles evaluation of carbon diffusion in Pd and Pd-based alloys*, Chen Ling and David S. Sholl, *Phys. Rev. B*, **80** (2009) 214202.
276. *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.
277. **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]
278. *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
279. **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.
280. *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.
281. ***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.
282. *Enantiospecific adsorption of amino acids on hydroxylated quartz(0001)*, Jeong Woo Han and David S. Sholl, *Langmuir*, **25** (2009) 10737-10745.

283. **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
284. ***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
285. *Selection of dopants to enhance hydrogen diffusion rates in MgH₂ and NaMgH₃*, Shiqiang Hao and David S. Sholl, Applied Physics Letters, **94** (2009) 171909.
286. ***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.
287. *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.
288. *Step decoration of chiral metal surfaces*, Jeong Woo Han, John Kitchin, and David S. Sholl, J. Chemical Physics, **130** (2009) 124710.
289. *First principles investigation of metal sulfides as membranes in hydrogen purification*, Chen Ling and David S. Sholl, J. Membrane Science, **329** (2009) 153-159.
290. ***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.
291. *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)
292. **Hydrogen diffusion in MgH₂ and NaMgH₃ via concerted motions of charged defects*, Shiqiang Hao and David S. Sholl, Applied Physics Letters, **93** (2008) 251901
293. *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.
294. ***Assessment of a metal-organic framework membrane for gas separations using atomically detailed calculations: CO₂, CH₄, N₂, H₂ mixtures in MOF-5*, Seda Keskin and David S. Sholl, Ind. Eng. Chem. Res. **48** (2009) 914-922.
295. **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.
296. *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.
297. *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.

298. *Atomistic simulations of CO₂ and N₂ 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.
299. ***Progress, opportunities, and challenges for applying atomically-detailed modeling to molecular adsorption and transport in metal-organic framework materials*, Seda Keskin, Jinchun Liu, Rees B. Rankin, J. Karl Johnson, and David S. Sholl, *Industrial and Engineering Chemistry Research*, **48** (2009) 2355-2371.
300. *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.
301. **Testing the accuracy of correlations for multi-component mass transport of adsorbed gases in metal organic frameworks: Diffusion of CH₄/H₂ mixtures in CuBTC*, Seda Keskin, Jinchun Liu, J. Karl Johnson, and David S. Sholl, *Langmuir*, **24** (2008) 8254.
302. *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.
303. **Combining Density Functional Theory and Cluster Expansion Methods to Predict H₂ Permeance Through Pd-based Binary Alloy Membranes*, Lymarie Semidey-Flecha and David S. Sholl, *J. Chem. Phys.*, **128** (2008) 144701
304. *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
305. *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.
306. *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.
307. **First principles study of experimental and hypothetical Mg(BH₄)₂ crystal structures*, Bing Dai, David S. Sholl, and J. Karl Johnson, *J. Phys. Chem. C*, **112** (2008) 4391-4395
308. *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
309. *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
310. *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.

311. ****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.
312. *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
313. *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
314. ***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
315. *Using first-principles calculations to predict surface resistances to H₂ transport through metal alloy membranes*, Chen Ling and David S. Sholl, *J. Membrane Sci.*, **303** (2007) 162
316. ****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
317. *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
318. *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
319. ***Experimental and Computational Prediction of the Hydrogen Transport Properties of Pd₄S**, 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
320. *Soaking It All Up (book review)*, David S. Sholl, *Materials Today*, **10** (2007) 61.
321. *Tuning Selectivity in Adsorption on Composite Chiral Surfaces*, Pawel Szabelski and David S. Sholl, *J. Phys. Chem. C*, **111** (2007) 11936-11942.
322. ***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.
323. *First principles investigation of adsorption and dissociation of hydrogen on Mg₂Si surfaces*, Bing Dai, David S. Sholl, and J. Karl Johnson, *J. Phys. Chem. C*, **111** (2007) 6910-6916.
324. *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
325. *Chiral separation on a model adsorbent with periodic surface heterogeneity*, Pawel Szabelski and David S. Sholl, *J. Chem. Phys.*, **126** (2007) 144709.
326. ****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)

327. *First principles screening of destabilized metal hydrides for high capacity H₂ storage using scandium*, Sudhakar V. Alapati, J. Karl Johnson, and David S. Sholl, *J. Alloys Compounds*, **446-447** (2007) 23-27.
328. **Using Density Functional Theory to Study Hydrogen Diffusion in Metals: A Brief Overview*, David S. Sholl, *J. Alloys Compounds*, **446-447** (2007) 462.
329. **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.
330. *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
331. **Influences of Interfacial Resistances on Gas Transport Through Carbon Nanotube Membranes*, David A. Newsome and David S. Sholl, *Nano Letters*, **6** (2006) 2150-2153.
332. *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.
333. *Atomically-detailed Simulations of Surface Resistances to Transport of CH₄, CF₄, and C₂H₆ through Silicalite Membranes*, David A. Newsome and David S. Sholl, *Micro. Meso. Materials*, **107** (2008) 286-295
334. *Dense Metal Membranes for Production of High Purity Hydrogen*, David S. Sholl and Y. H. Ma, *MRS Bulletin*, **31** (2006) 770-773
335. ***Making High-Flux Membranes with Carbon Nanotubes*, David S. Sholl and J. Karl Johnson, *Science*, **312** (2006), 1003 [Perspective Article]
336. *Testing Predictions of Macroscopic Binary Diffusion Coefficients Using Lattice Models with Site Heterogeneity*, David S. Sholl, *Langmuir*, **22** (2006) 3707-3714
337. *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
338. *Applications of Density Functional Theory to Heterogeneous Catalysis*, David S. Sholl, *Chemical Modelling: Applications and Theory*, **4** (2006) 108-160
339. ***Understanding Macroscopic Diffusion of Adsorbed Molecules in Crystalline Nanoporous Materials via Atomistic Simulations*, David S. Sholl, *Acc. Chem. Res.*, **39** (2006) 403-411.
340. ***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
341. *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
342. *Efficient simulation of binary adsorption isotherms using Transition Matrix Monte Carlo*, Haibin Chen and David S. Sholl, *Langmuir*, **22** (2006) 709-716
343. *Towards Computational Screening of Ternary Metal Alloys for Hydrogen Purification Membranes*, Preeti Kamakoti and David S. Sholl, *J. Membrane Sci.*, **279** (2006) 94-99.
344. **Enantiospecific Chemisorption of Small Molecules on Intrinsically Chiral Cu Surfaces*, Bhawna Bhatia and David S. Sholl, *Angew. Chemie Int. Ed.*, **44** (2005) 7761.

345. *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.
346. *Pt Thin Films on the Polar LaAlO₃(100) Surface: A First-Principles Study*, Aravind Asthagiri and David Sholl, *Phys. Rev. B*, **73** (2006) 125432
347. *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.
348. ***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
349. ***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
350. *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.
351. **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.
352. **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.
353. ***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.
354. *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. Tysoc, and David S. Sholl, *Catalysis Today*, **105** (2005) 74-77.
355. *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.
356. **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.
357. ***Predictions of selectivity and flux for CH₄/H₂ separations using single walled carbon nanotubes as membranes*, Haibin Chen and David S. Sholl, *J. Membrane Sci.*, **269** (2006) 152-160.
358. *Brownian Dynamics Study of Polymer-Stabilized Nanoparticles*, Abdulwahab Almusallam and David S. Sholl, *Nanotechnology*, **16** (2005) S409-S415.
359. **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.
360. *DFT Study of Pt adsorption on low index SrTiO₃ surfaces: SrTiO₃ (100), SrTiO₃ (111), SrTiO₃ (110)*, Aravind Asthagiri and David S. Sholl, *Surface Science*, **581** (2005) 66-87.

361. **Chemisorption and Diffusion of Hydrogen on Flat and Stepped Nickel Surfaces*, Bhawna Bhatia and David Sholl, J. Chem. Phys., **122** (2005) 204707.
362. ***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.
363. *Kinetics of H₂ desorption from C₆₀*, S. A. FitzGerald, R. Hannachi, D. Sethna, M. Rinkoski, Kurt K. Sieber, and David S. Sholl, Phys. Rev. B, **71** (2005) 045415.
364. **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.
365. **Structure of enantiopure and racemic alanine adlayers on Cu(110)*, Rees B. Rankin and David S. Sholl, Surf. Sci. Lett. **574** (2005) L1-L8
366. *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.
367. ***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.
368. **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.
369. *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.
370. *Diffusion of hydrogen in cubic Laves phase HfTi₂H_x*, Bhawna Bhatia, Xinjun Luo, C. A. Sholl, and David S. Sholl, J. Phys.:Condens. Matter. **16** (2004) 8891-8903
371. *Determination of concentration dependent transport diffusivity of CF₄ 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.
372. *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.
373. *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.
374. ***Rapid Diffusion of CH₄/H₂ Binary Mixtures in Carbon Nanotubes*, Haibin Chen and David S. Sholl, J. Am. Chem. Soc., **126** (2004) 7778-7779.
375. *Pt Thin Films on Stepped SrTiO₃ Surfaces: SrTiO₃(620) and SrTiO₃(622)*, Aravind Asthagiri and David S. Sholl, J. Mol. Catal. A, **216** (2004) 233-246.
376. *Density Functional Theory Studies of the Interaction of H, S, Ni-H, and Ni-S Complexes with MoS₂ Basal Plane*, Dan Sorescu, David S. Sholl, and Anthony V. Cugini, J. Phys. Chem. B, **108** (2004) 239-249
377. *Mechanisms and Rates of Interstitial H₂ Diffusion in Crystalline C₆₀*, Blas P. Uberuaga, Arthur F. Voter, Kurt Ken Sieber, and David S. Sholl, Physical Review Letters, **91** (2003) 105901.

378. ****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.
379. ****Correlation effects in diffusion of CH₄/CF₄ 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.
380. ***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.
381. **Comparing Atomistic Simulations and Experimental Measurements for CH₄/CF₄ 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.
382. ***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.
383. ****Chiral Selection on Inorganic Crystalline Surfaces**, Robert M. Hazen and David S. Sholl, *Nature Materials* **2** (2003) 367-374 (invited review article).
384. ****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.
385. ****Monte Carlo Simulation of Single- and Binary-Component Adsorption of CO₂, N₂, and H₂ in Zeolite Na-4A**, E. Demet Akten, Ranjani Siriwardane, and David S. Sholl, *Energy and Fuels*, **17** (2003) 977-983.
386. ****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.
387. ***Thin Pt films on the polar SrTiO₃(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.
388. **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.
389. **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].
390. ****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.
391. **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.
392. **First Principles Study of Adsorption and Diffusion of Ni and Ni-thiophene Complexes on MoS₂ Basal Planes**, Daniel Sorescu, David S. Sholl, and Anthony Cugini, *J. Phys. Chem. B.*, **107** (2003) 1988-2000.

393. **Atomistic Simulations of CO₂ and N₂ 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.
394. **First Principles Study of Pt Adhesion and Growth on SrO- and TiO₂-terminated SrTiO₃(100)*, Aravind Asthagiri and David S. Sholl, *J. Chem. Phys.*, **116** (2002) 9914-9925.
395. **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.
396. **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.
397. ***Transport Diffusivities of CH₄, CF₄, He, Ne, Ar, Xe, and SF₆ in Silicalite From Atomistic Simulations*, Anastasios I. Skoulidas and David S. Sholl, *J. Phys. Chem. B*, **106** (2002) 5058-5067.
398. ***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.
399. **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.
400. ***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.
401. ***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].
402. **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.
403. **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.
404. **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.
405. **Predicting Single-Component Permeance Through Macroscopic Zeolite Membranes from Atomistic Simulations*, David S. Sholl, *Industrial and Engineering Chemistry Research*, **39** (2000) 3737.
406. **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.

407. *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.
408. *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.
409. *Influences of Concerted Cluster Diffusion on Single File Diffusion of CF₄ in AlPO₄-5 and Xe in AlPO₄-31*, David S. Sholl and Cha Kun Lee, *Journal of Chemical Physics*, **112** (2000) 817.
410. *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).
411. ***Quantum Sieving in Carbon Nanotubes and Zeolites*, Qinyu Wang, Sivakumar Challa, David S. Sholl, and J. Karl Johnson, *Physical Review Letters* **82** (1999) 956.
412. *Characterization of Molecular Cluster Diffusion in AlPO₄-5 Using Molecular Dynamics*, David S. Sholl, *Chemical Physics Letters*, **305** (1999) 269.
413. *Characterizing Adsorbate Passage in Molecular Sieve Pores*, David S. Sholl, *Chemical Engineering Journal*, **74** (1999) 25.
414. *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.
415. ***A Generalized Surface Hopping Model*, David S. Sholl and John C. Tully, *Journal of Chemical Physics* **109** (1998) 7702.
416. *Reply to Comment on “Normal, Single-File, and Dual-Mode Diffusion of Binary Adsorbate Mixtures in AlPO₄-5”*, David S. Sholl and Kristen A. Fichthorn, *Journal of Chemical Physics* **109** (1998) 5693.
417. ***Adsorption of Chiral Hydrocarbons on Chiral Platinum Surfaces*, David S. Sholl, *Langmuir*, **14** (1998) 862.
418. **Concerted Diffusion of Molecular Clusters in a Molecular Sieve*, David S. Sholl and Kristen A. Fichthorn, *Physical Review Letters* **79** (1997) 3569.
419. **Normal, Single-File, and Dual-Mode Diffusion of Binary Adsorbate Mixtures in AlPO₄-5*, David S. Sholl and Kristen A. Fichthorn, *Journal of Chemical Physics* **107** (1997) 4384.
420. *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.
421. *Adsorption Kinetics of Chemisorption by Surface Abstraction and Dissociative Adsorption*, David S. Sholl, *Journal of Chemical Physics* **106** (1997) 289.
422. *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.
423. *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.
424. *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.
425. *Late Stage Coarsening of Adlayers by Dynamic Cluster Coalescence*, David S. Sholl and Rex T. Skodje, *Physica A* **231** (1996) 631.
426. *A Model Surface Reaction on Stepped Surfaces*, David S. Sholl and Rex T. Skodje, *Surface Science* **345** (1996) 173.
427. *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.
428. *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.
429. *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.
430. *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.
431. *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.
432. *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.
433. *Diffusion of Xenon on a Platinum Surface: The Influence of Correlated Flights*, David S. Sholl and Rex T. Skodje, *Physica D* **71** (1994) 168.
434. *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.
435. *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.
436. *Perturbative Calculation of Superperiod Recurrence Times in Nonlinear Chains*, David S. Sholl and B. I. Henry, *Physics Letters A* **159** (1991) 21.
437. *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.
438. *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 (2nd ed.), David S. Sholl and Jan Steckel, John Wiley & Sons, 2023 (ISBN: 978-1119840862).

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

- Turkish edition published in 2014.
- Japanese and Chinese editions published in 2015.
- > 2300 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. Plenary Lecture, Gordon Research Conference on Membranes: Materials and Processes, Colby-Sawyer College, New London, NH, July 2024
2. Plenary Panel, DOE Better Buildings Summit, Washington DC, April 2024
3. AI and Data Section, Computational Sciences Division, Oak Ridge National Laboratory, February 2024
4. Better Plants Technology Days, Oak Ridge National Laboratory, February 2024
5. ORNL Core Universities AI Workshop, Georgia Tech, Atlanta, GA, October 2023
6. Frontiers in Energy Technologies Workshop, University of Chicago, Chicago, IL, October 2023
7. University of Tennessee Postdoc Association, Knoxville, TN, September 2023
8. Department of Chemical Engineering, University of Alabama, Tuscaloosa, AL, September 2023
9. Direct Air Capture Technology Development – An Emerging Support Ecosystem Panel, FECM Carbon Management Review Meeting, Pittsburgh, PA, August 2023
10. Southeast Energy Policy Forum, Baker School of Public Policy and Public Affairs, University of Tennessee, Knoxville, TN, August 2023
11. Symposium on Enhancing Rigor and Reproducibility in Catalysis and Materials Chemistry, ACS National Meeting, San Francisco, CA, August 2023

12. BTSD/WINGS Career Forum: Long Term Career Vision and Shaping, Oak Ridge National Laboratory, Oak Ridge, TN, May 2023
13. Creating Good Ideas Workshop, Future Leaders and WiNS, Oak Ridge National Laboratory, Oak Ridge, TN, May 2023
14. 3M Tech Forum Climate Chapter, 3M Corporate Research, April 2023 (virtual)
15. University of the Third Age, Armidale, NSW, Australia, April 2023
16. Energy Systems Analysis Graduate Seminar, Department of Mechanical Engineering, University of Maryland, March 2023 (virtual)
17. Kurt Wohl Memorial Lecture, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, February 2023
18. University of Oklahoma Sustainability Forum, University of Oklahoma, Norman, OK, January 2023
19. Oak Ridge Public Library Tech Talk, Oak Ridge, TN, January 2023
20. Chemical Sciences. Geosciences and Biological Sciences seminar, Sandia National Laboratory (virtual), January 2023
21. Encouraging Creative Risk Taking in Your Students, Taylor & Francis Webinar, December 2022
22. Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, December 2022
23. Panel member, Influencing Policy Decisions on Climate Solutions, AIChE Annual Meeting, Phoenix, AZ, November 2022
24. Panel member, Powering The Future, AIChE Annual Meeting, Phoenix, AZ, November 2022
25. Panel member, Regeneration: Healing the Earth to End Climate Change, University of Tennessee Baker Center for Public Policy, Knoxville, TN, November 2022
26. Department of Chemical Engineering Graduate Student Symposium Keynote Talk, Carnegie Mellon University, Pittsburgh, PA, October 2022
27. National Energy Technology Laboratory, Pittsburgh, PA, October 2022
28. Gordon Conference on Chemical Separations, Ventura, CA, October 2022
29. University of Tennessee Science Forum, Knoxville, TN, September 2022
30. Department of Chemical Engineering, University of Queensland, August 2022 (virtual)
31. American Ceramic Society Young Professionals Network, Professional Skills and Personal Development Webinar Series, August 2022 (virtual)
32. Closing the Carbon Cycle Workshop, Pacific Northwest National Laboratory, Richland, WA, July 2022
33. Experience ORNL, Oak Ridge National Laboratory, Oak Ridge, TN, May 2022
34. Texas Tech University CheGSA Distinguished Speaker Series, Dept. of Chemical Engineering, Texas Tech University, April 2022 (virtual)
35. NSF/DOE Workshop on Addressing Rigor and Reproducibility in Heterogeneous Catalysis, April 2022 (virtual)
36. Department of Chemical Engineering, Pennsylvania State University, State College, PA, October 2021
37. Chemical Engineering Alumni Lectures, University of Massachusetts Amherst, September 2021

38. DOE Advanced Manufacturing Office TRANSFORM Initiative Workshop (virtual meeting), September 2021
39. NRL Workshop on Direct Air Capture and Blue Carbon Removal (virtual meeting), August 2021
40. Symposium on Surface Chemistry and Solvation Effects in Confined Environments, ACS Virtual National Meeting, April 2021
41. Virtual seminar, International Adsorption Society, March 2021
42. Plenary talk, North American Membrane Society 2020 Meeting (virtual meeting), May 2020
43. Department of Chemical and Environmental Engineering, University of Arizona, Tucson, AZ, October 2019
44. Dumas Lecture in Chemical Engineering, Department of Chemical Engineering, Virginia Tech, Blacksburg, VA, October 2019
45. Reproducibility in Science and Engineering, ACS 66th International Symposium, Columbus, OH, October 2019
46. Department of Chemical Engineering, Seoul National University, Seoul, South Korea, October 2019
47. Department of Chemical Engineering, Nanyang University, Singapore, October 2019
48. Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, October 2019
49. Department of Chemical and Biomolecular Engineering, University of Notre Dame, South Bend, IN, September 2019
50. Keynote Lecture, DOE BES Separations PI Meeting, Gaithersburg, MD, September 2019
51. School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ, September 2019
52. School of Chemical & Biomolecular Engineering, Georgia Tech, August 2019
53. Gordon Research Conference on Nanoporous Materials, Andover, NH, August 2019
54. Department of Chemical Engineering, New Mexico State University, Las Cruces, NM, April 2019
55. Department of Chemical Engineering, University of Arkansas, April 2019
56. Symposium on New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations and Theory, ACS National Meeting, Orlando, FL, March 2019
57. George Olah Award Symposium in Honor of Chunshan Song, ACS National Meeting, Orlando, FL, March 2019
58. Department of Chemical Engineering, University of New Hampshire, Durham, NH, March 2019
59. Ma Lecture, Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA, March 2019
60. Physical Sciences Division, Pacific Northwest National Laboratory, Richland, WA, March 2019
61. Department of Chemical Engineering, Oklahoma State University, Stillwater, OK, December 2018
62. University College London, London, UK, December 2018

63. Department of Chemical Engineering, Virginia Commonwealth University, Richmond, VA, October 2018
64. Department of Chemical Engineering, Drexel University, Philadelphia, PA, November 2018
65. Department of Chemical Engineering and Materials Science, University of Alberta, Edmonton, Alberta, October 2018
66. Parr Lecture, Department of Chemical and Biomolecular Engineering, University of Illinois, Champaign, IL, September 2018
67. Plenary Lecture, 15th International Conference on Inorganic Membranes, Dresden, Germany, June 2018
68. Department of Nanoengineering, UCSD, La Jolla, CA, April 2018
69. Department of Chemical Engineering, UC Berkeley, Berkeley, CA, March 2018
70. Department of Chemical Engineering, South Dakota School of Mines, March 2018
71. Plenary Lecture, 2018 US DOE Basic Energy Sciences Separation Science PI Meeting, Gaithersburg, MD, February 2018
72. Material Informatics Seminar, National Institute of Standards, Gaithersburg, MD, February 2018
73. New Vistas in Molecular Thermodynamics, Humboldt Kolleg, Berkeley, CA, January 2018
74. NAS Committee on Reproducibility and Replicability in Science, Washington DC, December 2017
75. Sustainable Engineering Forum Plenary Session, AIChE Annual Meeting, Minneapolis, MN, November 2017
76. Department of Chemical Engineering, MIT, Boston, MA, October 2017
77. Department of Chemical Engineering, Tulane University, New Orleans, LA, September 2017
78. Department of Chemical Engineering, Kansas State University, Manhattan, KS, September 2017
79. Department of Chemical & Petroleum Engineering, University of Kansas, Lawrence, KS, September 2017
80. Sandia National Laboratory, Albuquerque, NM, August 2017
81. ORNL Materials Informatics Workshop, Oak Ridge National Lab, Oak Ridge, TN, August 2017
82. ASEE Summer School for Chemical Engineering Faculty, Raleigh, NC, August 2017
83. Keynote Lecture, Australian CCS Research Conference, Melbourne, VIC, Australia, June 2017
84. AINST Distinguished Seminar, University of Sydney, Sydney, NSW, Australia, June 2017
85. Department of Chemical Engineering, University of New South Wales, Kensington, NSW, Australia, June 2017
86. Department of Physics Colloquium, University of Queensland, Brisbane, QLD, Australia, June 2017
87. CSIRO and University of Monash Department of Chemistry, Clayton, VIC, Australia, May 2017
88. Mieryngah Public Lecture, University of Melbourne, Melbourne, Australia, May 2017

89. Tau Beta Pi Initiates Dinner talk, Georgia Institute of Technology, Atlanta, GA, April 2017
90. Department of Chemical Engineering, University of California Davis, Davis, CA, March 2017
91. Department of Chemical Engineering, Colorado School of Mines, Golden, CO, January 2017
92. Robin H. Stokes Lecture, University of New England, Armidale, NSW, Australia, December 2016
93. Plenary Lecture, Fundamentals and Applications of Advanced Porous Materials Conference, Adelaide, South Australia, Australia, December 2016
94. Department of Chemical and Biological Engineering, University of Delaware, Newark, DE, December 2016
95. Department of Chemical Engineering and Materials Science, Cal Poly Pomona, Pomona, CA, November 2016
96. Department of Chemical Engineering, Texas Tech, Lubbock, TX, November 2016.
97. Georgia Research Alliance Eminent Scholars Annual Meeting, Atlanta, GA, October 2016.
98. Symposium on Supramolecular Assemblies and Metal-Organic Frameworks, SERMACS, Columbia, SC, October 2016.
99. University of Houston Honors College, Houston, TX, October 2016
100. School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, September 2016
101. Department of Chemical Engineering, University College Dublin, Dublin, Ireland, September 2016
102. International Zeolite Membrane Meeting 2016, Dalian, China, August 2016
103. University of Seoul, Seoul, Korea, August 2016
104. Seoul National University, Seoul, Korea, August 2016
105. Board for Chemical Sciences and Technology, National Academy of Sciences, Irvine, CA, August 2016.
106. Gordon Conference on Membranes, New London, NH, August 2016.
107. Gulf Coast and Latin America Scientists Association Seminar Series, Dow Chemical, Freeport, TX, May 2016
108. Savannah River National Laboratory, Aiken, SC, May 2016
109. Symposium on Design, Synthesis and Applications of Advanced Porous Materials, Pacifichem, Honolulu, HI, December 2015
110. Symposium on Data Mining and Machine Learning Meets Experiment and First-principles Simulation for Materials Discovery, Pacifichem, Honolulu, HI, December 2015
111. Symposium on Safety in the Academic Research Laboratory, Pacifichem, Honolulu, HI, December 2015
112. Department of Chemical, Petroleum and Materials Engineering, University of Southern California, Los Angeles, CA, October 2015
113. Department of Chemical and Biomolecular Engineering, University of California Riverside, Riverside, CA, October 2015
114. Department of Chemical and Biomolecular Engineering, University of California Irvine, Irvine, CA, October 2015

115. Department of Chemical Engineering, University of Houston, Houston, TX, October 2015
116. Department of Chemical and Biomolecular Engineering, University of Florida, Gainesville, FL, September 2015
117. Department of Chemical and Biological Engineering, University of Buffalo, Buffalo, NY, September 2015
118. Department of Chemical Engineering, Northeastern University, Boston, MA, August 2015
119. Multiscale Porosity From Laboratory To Industrial Application, 2nd Micromeritics Workshop, Massachusetts Institute of Technology, Cambridge, MA, August 2015
120. School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, August 2015
121. US-Korea Conference on Science, Technology, and Entrepreneurship , Atlanta, GA, July 2015
122. DOE BES Catalysis Contractors Workshop, Annapolis, MD, July 2015
123. Gordon Research Conference on Hydrogen Metal Systems, Stonehill College, MA, July 2015
124. Workshop on Metal-Organic Frameworks, Telluride Scientific Research Conference, Telluride, CO, June 2015.
125. CECAM Workshop on Defects and Disorder in Metal-Organic Frameworks, Chimie ParisTech, Paris, France, June 2015
126. 3M Tech Talk, Minneapolis, MN, May 2015
127. UOP Technical Seminar, Des Plaines, IL, May 2015
128. Department of Chemical Engineering, University of Illinois at Chicago, Chicago, IL, May 2015
129. Symposium on Genomic Approaches to Materials, 249th ACS National Meeting, Denver, CO, March 2015
130. Symposium on Environmental Applications of Metal-Organic Frameworks, 249th ACS National Meeting, Denver, CO, March 2015
131. Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, March 2015
132. Department of Chemical and Biomolecular Engineering, University of South Florida, Tampa, FL, February 2015
133. Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD, December 2014
134. Chinese American Chemical Society Banquet, Atlanta, GA, November 2014
135. Molecular Thermodynamics Plenary Session, AIChE Annual Meeting, Atlanta, GA, November 2014
136. Fossil Fuels Plenary Session, AIChE Annual Meeting, Atlanta, GA, November 2014
137. Department of Chemical and Biomolecular Engineering, Columbia University, New York, NY, November 2014
138. Adsorption Technologies Group, Sasol, Sasolburg, South Africa, November 2014
139. Particle Technology Workshop, University of Cape Town, Cape Town, South Africa, November 2014
140. ExxonMobil Applied Materials Symposium, Hershey, PA, October 2014

141. Department of Chemical and Biomolecular Engineering, University of Colorado, Boulder, CO, October 2014
142. Trotter Distinguished Lecture, Department of Chemical Engineering, University of Tennessee, October 2014
143. Symposium on MOFs for Applications, 248th ACS National Meeting, San Francisco, CA, August 2014
144. School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, August 2014
145. Metal Hydrogen 2014, Manchester, UK, July 2014
146. Department of Chemical Engineering, Imperial College London, London, UK, July 2014
147. Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, July 2014
148. Department of Chemistry, National University of Singapore, Singapore, July 2014
149. Department of Chemical Engineering, University of Melbourne, Melbourne, Australia, June 2014
150. International Conference on Inorganic Membranes (keynote address), Brisbane, Australia, June 2014
151. MRS Spring Meeting, San Francisco, CA, April 2014
152. Florida AVS Meeting, Orlando, FL, March 2014
153. J. H. Hopps 5th Annual Training Symposium, Morehouse College, Atlanta, GA, February 2014
154. Dow Chemical Company, Freeport, TX, January 2014
155. School of Chemistry Colloquium, Georgia Institute of Technology, Atlanta, GA, October 2013
156. Physical Chemistry Seminar, University of Wisconsin, Madison, WI, October 2013
157. Department of Chemical and Biomolecular Engineering, Northwestern University, Evanston, IL, October 2013
158. International Zeolite Membrane Meeting, Jeju Island, South Korea, June 2013
159. Workshop on Adsorption in Compliant Solids, Paris, France, June 2013
160. International Conference on Energy and Sustainability, Hang Zhou, China, May 2013
161. Department of Physics, Oberlin College, Oberlin, OH, May 2013
162. Symposium on CO₂ Capture and Utilization, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013
163. Symposium on Hydrogen Production, Storage, and Utilization, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013
164. Symposium on Identification of Environmental Abiotic and Biotic Reactions Using Computational Chemistry, (invited talk) 245th ACS National Meeting, New Orleans, LA, March 2013
165. Department of Chemistry, University of Florida, February 2013
166. Georgia Tech Clean Energy Speaker Series, Atlanta, GA, February 2013
167. CSIRO, Clayton, Victoria, Australia, December 2012
168. Dept. of Chemical Engineering, University of Queensland, December 2012
169. Pacific Northwest National Laboratory, December 2012

170. Department of Chemical Engineering, Clemson University, November 2012
171. Physical Chemistry seminar, Department of Chemistry, University College London, London, UK, October 2012
172. Air Capture: Developing Technologies for Carbon Recycling and Negative Emissions, Institution of Mechanical Engineering, London, UK, October 2012
173. MOF2012 Keynote Lecture, Edinburgh, UK, September 2012
174. Foundations of Molecular Modeling and Simulations, Portland, OR, July 2012.
175. NETL ORD Seminar, National Energy Technology Laboratory, Pittsburgh, PA, June 2012.
176. Symposium on Gas Capture Materials, Canadian Society of Chemistry Conference, Calgary, AB, May 2012
177. CNMS Theory Seminar, Oak Ridge National Laboratory, Oak Ridge, TN, May 2012
178. ORNL Reactor Off Gas Group, Oak Ridge National Laboratory, Oak Ridge, TN, May 2012
179. Washington University in St. Louis, Department of Energy, Environment, and Chemical Engineering, April 2012
180. University of South Carolina, Department of Chemical Engineering, Columbia, SC, March 2012
181. Materials Modeling Group, Intel Corporation, Santa Clara, CA, March 2012
182. Symposium on Non-adiabatic Dynamics: Surface Hopping and Beyond (invited talk), 243rd ACS National Meeting, San Diego, CA, March 2012
183. Symposium on High-Throughput Screening Approaches for Catalysts Discovery and Optimization (invited talk), 243rd ACS National Meeting, San Diego, CA, March 2012
184. University of California Berkeley, Carbon Capture Program, February 2012
185. Stanford University, Department of Energy Resources Engineering, February 2012
186. MADE@GT Symposium on Materials Design, Atlanta, GA, November, 2011
187. Georgia Research Alliance Eminent Scholars Annual Meeting, Atlanta, GA, October 2011
188. Department of Chemical Engineering Seminar, University of Kentucky, Louisville, KY, October 2011.
189. Sandia National Laboratory, Microfluidics Department, Livermore, CA, September 2011.
190. Nanoporous Materials VI (plenary presentation), Banff, Canada, August 21-24, 2011.
191. National Summit on Advancing Clean Energy Technologies (invited panelist), Washington DC, May 2011.
192. Workshop on Materials Design in Chemical Compound Space, Institute for Pure and Applied Mathematics, UCLA, Los Angeles, CA, May 2011
193. Symposium on Applications of Metal-Organic Frameworks, MRS Spring Meeting, San Francisco, CA, April 2011
194. APS March Meeting, Dallas, TX, March 2011
195. Department of Chemical Engineering, National University of Singapore, Singapore, February 2011

196. Institute for Atom-efficient Chemical Transformations Workshop, Northwestern University, Evanston, IL, November 2010
197. COMSEF Plenary Session, AIChE Annual Meeting, Salt Lake City, November 2010
198. Open Forum of the Energy and Environment, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, October 2010
199. Neutrons in Catalysis Workshop, Oak Ridge National Laboratory, September 2010
200. Symposium on Nanoporous Materials for Environmental Applications, ACS National Meeting, Boston, August 2010
201. 5th International Zeolite Membrane Meeting, Loutraki, Greece, May 2010.
202. Department of Chemical and Bioengineering, University of Washington, Seattle, WA, May 2010.
203. Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, April 2010.
204. Department of Chemical Engineering, The Pennsylvania State University, State College, PA, April 2010.
205. Keynote Lecture, Symposium on Advances in Membrane Science and Technology, ACS National Meeting, San Francisco, March 2010.
206. Dept. of Chemical Engineering, Texas A&M University, College Station, TX, January 2010.
207. Oak Ridge National Laboratory, Computational Materials Division, Knoxville, TN, January 2010.
208. Thin Films Division, AVS 56th International Symposium, San Jose, November 2009.
209. Dept. of Chemical Engineering, Clemson University, October 2009.
210. DOE Computational Materials Science Network Workshop, Denver, CO, October, 2009.
211. XVIII International Materials Research Congress, Cancun, Mexico, August 2009.
212. US-China Workshop on Surface Science and Heterogeneous Catalysis, Dalian, China, June 2009.
213. Savannah River National Laboratory, Materials Division, Aiken, SC, June 2009.
214. Swedish-American Entrepreneurial Days, Keynote Address, Savannah, GA, April 2009.
215. Emerson Center Annual Symposium, Emory University, March 2009.
216. Dept. of Chemical Engineering, University of Louisville, Louisville, KY, February 2009
217. Center for Simulational Physics, 22nd Annual Workshop, University of Georgia, Athens, GA, February 2009
218. Dept. of Chemical Engineering, University of New South Wales, Sydney, NSW, Australia, December 2008.
219. Dept. of Physics, University of Sydney, Sydney, NSW, Australia, December 2008.
220. Dept of Chemical Engineering, University of Melbourne, Melbourne, Victoria, Australia, December 2008

221. CSIRO Energy Research Center, Brisbane, Queensland, Australia, December 2008
222. Future Directions in Transport, Centennial Symposium, AIChE Annual Meeting, Philadelphia, November 2008.
223. Department of Chemical Engineering, University of Maine, Bangor, ME, October 2008
224. University of Queensland Physics Summer School, Stradbroke Island, Queensland, Australia, December 2008.
225. Center for Nanoscale Materials, Argonne National Laboratory, Chicago, IL, October 2008
226. Center for Simulational Physics, University of Georgia, Athens, GA, October 2008
227. College of Engineering, Peking University, Beijing, China, May 2008.
228. Department of Chemistry, Tsinghua University, Beijing, China, May 2008.
229. Department of Chemical Engineering, Beijing University of Chemical Technology, Beijing, China, May 2008.
230. Department of Chemistry, Emory University, Atlanta, GA, April 2008.
231. Thermodynamics in Chemical Engineering: Prospects and Perspectives, AIChE Spring Meeting, New Orleans, LA, April 2008.
232. Computational Methods and Molecular Modeling in Fuel Chemistry, ACS National Meeting, New Orleans, LA, April 2008.
233. Arthur W. Adamson Award for Distinguished Service of Surface Chemistry: Symposium in Honor of Francisco Zaera, ACS National Meeting, New Orleans, LA, April 2008.
234. Department of Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ, November 2007.
235. Department of Materials Science and Engineering, University of Illinois, Champaign, IL, November 2007.
236. MESD Plenary Session, AIChE Annual Meeting, Salt Lake City, UT, November 2007.
237. CECAM Workshop on Chirality at Surfaces, Lyons, France, October 2007.
238. Symposium on Advanced Materials for Conversion and Separations in Energy Applications, ACS National Meeting, Boston, MA, August 2007.
239. Symposium on Hydrogen Storage and Fuel Cell Technology, ACS National Meeting, Boston, MA, August 2007.
240. Gordon Conference on Hydrogen in Metals, Waterville, Maine, July 10, 2007.
241. Department of Chemical Engineering, Oklahoma University, April 19, 2007
242. Symposium on Capturing Complexity in Physical Sciences Simulation, ACS National Meeting, Chicago, IL, March 27, 2007
243. Symposium on Implications and Applications of Chirality in Physical Chemistry, ACS National Meeting, Chicago, IL, March 28, 2007
244. Department of Chemical Engineering and Materials Science, University of Minnesota, January 23, 2007.
245. Department of Chemistry, Carleton College, January 12, 2007.
246. Biosecurity and Nanosciences Laboratory, Lawrence Livermore National Laboratory, January 10, 2007.

247. COMSEF Plenary Session, AIChE Annual Meeting, San Francisco, California, November 12-16, 2006
248. Department of Chemical Engineering, Carnegie Mellon University, November 2, 2006
249. Department of Chemical Engineering, Vanderbilt University, October 30, 2006.
250. Department of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia, October 18, 2006
251. Metal-Hydrogen 2006, Maui, Hawaii, October 1-6, 2006
252. Symposium on Challenges for the Hydrogen Economy: Storage Science and Technology, ACS National Meeting, San Francisco, California, September 10-14, 2006.
253. Symposium on Chirality and Enantioselectivity at Surfaces, ACS National Meeting, San Francisco, California, September 10-14, 2006.
254. Symposium on Computational Materials Design in Chemical Industries, ACS National Meeting, San Francisco, California, September 10-14, 2006.
255. Gordon Research Conference on Membranes: Materials and Processes, New London, NH, August 6-11, 2006.
256. Gordon Research Conference on Physical Metallurgy, Plymouth, NH, July 23-26, 2006.
257. Gordon Research Conference on Chemistry at Interfaces, Biddeford, Maine, July 9-14, 2006.
258. Department of Physics, University of Sydney, Sydney, NSW, Australia, May 19, 2006.
259. 135th TMS Annual Meeting, March 12-16, 2006, San Antonio, TX.
260. Center for Low Emission Technologies, University of Queensland, Brisbane Australia, December 2005.
261. ARC Center for Functional Nanomaterials 2nd Annual Meeting, Noosa Heads, Australia, December 2005.
262. Department of Chemical Engineering, University of Melbourne, Melbourne, Australia, November 2005.
263. Center for Molecular Modeling, Swinburne University, Melbourne, Australia, November 2005.
264. China/Japan/USA Joint Chemical Engineering Meeting, Beijing, China, October 11-13, 2005.
265. Department of Chemical Engineering, University of Newcastle, Newcastle, Australia, October 2005.
266. CSIRO Energy Center, Newcastle, Australia, October 2005.
267. ExxonMobil Corporate Research, Annandale, NJ, October 2005.
268. Nanoscale Science and Technology Center, Griffith University, Brisbane, Australia, August 2005.
269. Department of Chemical Engineering and Materials Science, Arizona State University, Tempe, AZ, April 2005.
270. Department of Chemical Engineering, City College of New York, New York, NY, February 2005.
271. Department of Materials Science, University of Pittsburgh, Pittsburgh, PA, February 2005.

272. Department of Chemical Engineering, University of Colorado, Boulder, CO, January 2005.
273. Workshop on Molecular and Particle Processes at Solid Surfaces, San Luis, Argentina, November 2004.
274. ExxonMobil Corporate Research, Annandale, NJ, September 2004.
275. 3rd International Zeolite Membrane Meeting, Breckenridge, CO, July 2004.
276. van't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, Holland, May 2004.
277. Surface Science Center, University of Liverpool, Liverpool, UK, May 2004.
278. Department of Chemistry, University of Cardiff, Cardiff, UK, May 2004.
279. Department of Chemistry, University of Sydney, Sydney, NSW, Australia, May 2004.
280. Department of Physics, University of New England, Armidale, NSW, Australia, May 2004.
281. Department of Chemical Engineering, University of Queensland, Brisbane, Qld., Australia, April 2004.
282. Department of Chemical Engineering, Purdue University, West Lafayette, IN, March 2004.
283. Third San Luis Symposium on Surface Science, Merida, Venezuela, March 2004.
284. Department of Chemistry, Wake Forest University, Winston-Salem, NC, February 2004.
285. Department of Chemistry, Duquesne University, Pittsburgh, PA, January 2004.
286. Surface Analysis session, FACSS 2003 Annual Meeting, Ft. Lauderdale, FL, October 2003.
287. Department of Materials Science and Engineering, University of Florida, Gainesville, FL, October 2003.
288. Department of Chemical Engineering, University of Florida, Gainesville, FL, October 2003.
289. Department of Chemical Engineering, University of Buffalo, Buffalo, NY, October 2003.
290. CECAM Workshop on Simulation of Zeolites: Towards In Silico Design, Lyons, France, October 2003.
291. Department of Physics, Indiana University of Pennsylvania, Indiana, PA, September 2003.
292. Chiral Surfaces Symposium, ACS National Meeting, New Orleans, LA, March 2003.
293. Mechanistic Surface Chemistry Symposium, ACS National Meeting, New Orleans, LA, March 2003.
294. Department of Chemical Engineering, University of Missouri at Rolla, January 2003.
295. Pittsburgh-Cleveland Catalysis Society, Pittsburgh, PA, December 2002.
296. Department of Chemical Engineering, University of Wisconsin, December 2002.
297. CAST Plenary Session, AIChE Annual Meeting, Indianapolis, IN, November 2002.
298. Department of Chemical Engineering, University of Delaware, October 2002.
299. Pittsburgh AIChE Chapter, October 2002.

300. Materials Research Seminar, Department of Chemical Engineering, The Pennsylvania State University, October 2002.
301. Chemical Physics/Physical Chemistry Seminar, Departments of Chemistry and Physics, University of Maryland, September 2002
302. GE Corporate Research and Development, Albany, NY, September 2002
303. TDA Inc., Wheatridge, CO, June 2002.
304. National Renewable Energy Laboratory, June 2002.
305. Computational Materials and Biology Group, Sandia National Laboratory, Albuquerque, NM, June 2002.
306. Atomic and Molecular Physics Group, T-Division, Los Alamos National Laboratory, May 2002.
307. Department of Chemical Engineering, University of Massachusetts – Amherst, April 2002.
308. Department of Chemical Engineering, University of Akron, February 2002.
309. Air Products R&D Division, January 2002.
310. Department of Chemical Engineering, University of California at Santa Barbara, Santa Barbara, CA, November 2001.
311. Department of Chemistry, Kent State University, Kent, OH, September 2001.
312. Midwest Thermodynamics and Statistical Mechanics Meeting, East Lansing, MI, May 2001.
313. Computational Materials and Biology Group, Sandia National Laboratory, Albuquerque, NM, December 2000.
314. Department of Chemical Engineering, University of Colorado, October 2000.
315. Department of Applied Mathematics, University of Colorado, October 2000.
316. ExxonMobil Corporate Research Division, Annandale, NJ, June 2000.
317. Air Products and Chemicals Technology Division, Allentown, PA, June 2000.
318. Department of Chemical Engineering, University of Tennessee, April 2000.
319. ACS National Meeting, San Francisco, CA, March 2000 (invited presentation).
320. Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA, October 1999.
321. Condensed Matter Seminar, Department of Physics, Carnegie Mellon University, Pittsburgh, PA, October 1998
322. Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, PA, September 1998
323. Department of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, March 1997.
324. Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA, February 1997.
325. Department of Chemistry, Iowa State University, Ames, IA, January 1997.
326. Department of Applied Mathematics, University of Colorado, Boulder, CO, November 1995.
327. Physics Department, University of New England, Armidale, NSW, Australia, December 1993.
328. Department of Physics and Theoretical Physics, Australian National University, Canberra, ACT, Australia, March 1991.

Other Presentations (selected)

1. AIChE Annual Meeting, Pittsburgh, PA, October 2018 (12 contributed presentations and 2 posters)
2. AIChE Annual Meeting, Minneapolis, MN, October 2017 (12 contributed presentations)
3. AIChE Annual Meeting, San Francisco, CA, November 2016 (5 contributed presentations)
4. AIChE Annual Meeting, Salt Lake City, UT, November 2015 (2 contributed presentations)
5. AIChE Annual Meeting, Atlanta, GA, November 2015 (14 contributed presentations)
6. International Conference on Inorganic Membranes, Brisbane, Australia, June 2014 (1 contributed presentation)
7. Nano-7, Niagara Falls, Ontario, June 2014 (1 contributed presentation)
8. AIChE Annual Meeting, San Francisco, CA, November 2013 (8 contributed presentations)
9. AIChE Annual Meeting, Pittsburgh, PA, October 2012 (9 contributed presentations)
10. 243rd ACS National Meeting, San Diego, CA, March 2012 (1 contributed presentations, 1 invited presentation given by G. Parkinson)
11. 17th Symposium on Separation Science and Technology for Energy Applications, Nashville, TN, October 2011 (2 contributed presentation)
12. AIChE Annual Meeting, Minneapolis, MN, October 2011 (7 contributed presentations)
13. ACS National Meeting, Denver, CO, August 2011 (1 invited presentation given by K. Walton)
14. Gordon Conference on Nanoporous Materials (2 posters)
15. North American Membrane Society Meeting, Las Vegas, NV, June 2011 (2 contributed presentations)
16. MRS Spring Meeting, San Francisco, CA, April 2011 (1 contributed presentation)
17. ACS National Meeting, Anaheim, CA, March 2011 (3 contributed presentations)
18. AIChE Annual Meeting, Salt Lake City, UT, November 2010 (4 contributed presentations)
19. NETL CO₂ Technology Meeting, Pittsburgh, PA, September 2010 (1 poster)
20. MOF2010, Marseille, France, September 2010 (1 contributed presentation, 1 poster)
21. ACS National Meeting, Boston, MA, August 2010 (3 contributed presentations)
22. ACS National Meeting, San Francisco, CA, March 2010 (2 contributed presentations)
23. 13th IACS International Conference on Surface and Colloid Science, New York, NY, June 2009 (1 contributed presentation)
24. NAMS 2009, Charleston, SC, June 2009 (2 contributed presentations)
25. ACS National Meeting, Salt Lake City, UT, March 2009 (2 contributed presentations)
26. APS March Meeting, Pittsburgh, PA, March 2009 (3 contributed presentations)
27. MRS Fall Meeting, Boston, MA, December 2008 (1 contributed presentation)
28. AIChE Annual Meeting, Philadelphia, PA, November 2008 (8 contributed presentations)
29. ASME Energy Nanotechnology Meeting, Jacksonville, FL, August 2008 (1 contributed presentation)

30. Metal Hydrogen 2008, Reykjavik, Iceland, June 2008 (2 contributed presentations, 1 poster)
31. ACS National Meeting, New Orleans, LA, April 2008 (1 contributed presentation)
32. National Hydrogen Association Annual Meeting, Sacramento, CA, March 2008 (1 contributed presentation, 1 poster)
33. ACS National Meeting, Boston, MA, August 2007 (7 contributed presentations)
34. North American Membrane Society Annual Meeting, Orlando, FL, May 14-16, 2007 (2 contributed presentations)
35. PCCS Spring Meeting, Morgantown, WV (3 contributed presentations)
36. 2nd International Workshop on In-situ Study and Development of Processes Involving Porous Materials, Thessalonika, Greece, February 24-28, 2007 (poster)
37. AIChE Annual Meeting, November 2006, San Francisco, CA (3 contributed presentations)
38. Metal-Hydrogen 2006, Maui, Hawaii, October 1-6, 2006 (contributed presentation)
39. 2006 Midwest Thermodynamics and Statistical Mechanics Meeting, Akron, OH, May 25-26, 2006 (3 presentations)
40. PCCS Fall Meeting, Pittsburgh, PA, December 9, 2005
41. China/Japan/USA Joint Chemical Engineering Meeting, Beijing, China, October 11-13, 2005 (contributed presentation)
42. W. E. Heraeus Seminar on Hydrogen Storage with Novel Nanomaterials, Bad Honnef, Germany, 23-27 October, 2005
43. ACS National Meeting, Washington, DC, August 28-September 1, 2005 (1 presentation, 2 posters)
44. Gordon Conference on Zeolitic and Layered Materials, South Hadley, MA, July 3-8, 2005 (poster).
45. 2005 Midwest Thermodynamics and Statistical Mechanics Meeting (3 presentations)
46. 19th North American Catalysis Society Meeting, Philadelphia, PA, May 22-27, 2005
47. PCCS Spring Meeting, Pittsburgh, PA, June 2005 (3 presentations)
48. ACS National Meeting, San Diego, CA, March 2005.
49. AIChE Annual Meeting, Austin, TX, November 2004 (7 presentations)
50. 2004 ASM Materials Solutions Conference, Columbus, OH, October 18-20, 2004.
51. 8th International Conference on Inorganic Membranes, Cincinnati, OH, June 2004 (4 presentations)
52. PCCS Spring Meeting, Pittsburgh, PA, June 2004 (2 presentations).
53. 2004 Midwest Thermodynamics and Statistical Mechanics Meeting (3 presentations).
54. ACS National Meeting, Anaheim, CA, March 2004 (4 presentations).
55. APS March Meeting, Montreal, Canada, March 2004.
56. AVS 50th International Symposium, Baltimore, MD, November 2003.
57. AIChE 2003 Annual Meeting, San Francisco, CA, November 16-21, 2003 (5 presentations)
58. 63rd Physical Electronics conference, Ithaca, NY, June 16-18, 2003.
59. 2003 Midwest Thermodynamics and Statistical Mechanics Meeting, Columbus, OH May 28-29, 2003 (3 presentations)
60. 2003 North American Membrane Society Meeting, Jackson Hole, WY, May 19-21, 2003 (2 presentations)
61. NASA Astrobiology General Institute Meeting, Tempe, AZ, Feb 10-12, 2003.

62. AIChE National Meeting, Indianapolis, IN, November 3-8, 2002 (7 presentations)
63. AVS 49th International Symposium, Denver, CO, November 3-8, 2002 (2 presentations)
64. ACS National Meeting, Boston, MA, August 17-21, 2002
65. American Conference on Theoretical Chemistry, Champion, PA, July 13-18, 2002 (2 posters)
66. 62nd Physical Electronics conference, Atlanta, GA, June 12-14, 2002.
67. 2002 Midwest Thermodynamics and Statistical Mechanics Meeting, Pittsburgh, PA, May 13-14, 2002 (4 presentations)
68. 2002 Pittsburgh-Cleveland Catalysis Society Symposium, Pittsburgh, PA, May 9-10, 2002 (2 presentations)
69. ACS National Meeting, Orlando, FL, April 7-11, 2002 (3 presentations)
70. APS March Meeting, Indianapolis, IN, March 18-22, 2002 (3 presentations)
71. AIChE National Meeting, Reno, NV, November 4-9, 2001 (4 presentations)
72. International Workshop on Zeolitic and Microporous Membranes, Purend, The Netherlands, July 2001 (poster).
73. 7th International Conference on Fundamentals of Adsorption, Nagasaki, Japan, May 20-25, 2001.
74. North American Membrane Society Annual Meeting, Lexington, KY, May 2001.
75. ACS Surfaces and Colloids Symposium, Pittsburgh, PA, June 2001 (2 presentations)
76. 2001 Midwest Thermodynamics and Statistical Mechanics Meeting, East Lansing, MI, May 2001.
77. MRS Spring Meeting, San Francisco, CA, April 2001 (3 presentations)
78. ACS National Meeting, San Diego, CA, March 2001 (3 presentations)
79. AIChE National Meeting, Los Angeles, CA, November 2000 (3 presentations).
80. ACS Colloids and Surfaces Symposium, Lehigh, PA, June 2000 (3 presentations)
81. Access in Nanoporous Materials II, Banff, Alberta, May 2000 (1 presentation & 1 poster)
82. 2000 Midwest Thermodynamics and Statistical Mechanics Meeting, Minneapolis, MN, May 2000.
83. ACS national meeting (3 presentations), San Francisco, CA, March 2000.
84. Workshop on Nanotribology: Critical Assessment and Research Needs, Gaithersburg, MD, March 2000 (poster).
85. AIChE National Meeting (6 presentations), Dallas, TX, November 1999.
86. Nanotube '99, Michigan State University, Lansing, MI, July 1999 (poster).
87. Joint US/German Workshop on Ultrasensitive Chemistry and Engineering, New Orleans, LA, August 1999 (2 posters).
88. ACS Surfaces and Colloids Symposium (2 presentations), MIT, Boston, MA, June 1999
89. American Conference on Theoretical Chemistry (poster), Boulder, CO, July 1999.
90. Colloids, Polymers and Surfaces Program Mini-symposium, Carnegie Mellon University, Pittsburgh, PA, May 1999.
91. 1999 Midwest Thermodynamics and Statistical Mechanics Conference (2 presentations), Detroit, MI, May 1999
92. Zeolite Membrane Research Group, Chemical Engineering Department, University of Colorado, Boulder, CO, May 1999

93. MRS Fall Meeting, Boston, MA, December 1998.
94. AIChE National Meeting (2 presentations), Miami, FL, November 1998
95. AVS National Symposium, Baltimore, MD, November 1998
96. ACS Surfaces and Colloids Symposium, State College, PA, June 1998.
97. 1998 Midwest Thermodynamics and Statistical Mechanics Conference, Notre Dame, IN, May 1998.
98. AIChE National Meeting, Los Angeles, CA, November 1997 (2 presentations).
99. Materials Science in Chemical Engineering seminar, Department of Chemical Engineering, Pennsylvania State University, State College, PA, January 1997.
100. AIChE National Meeting, Chicago, IL, November 1996 (2 presentations)
101. AVS National Symposium, Philadelphia, PA, October 1996.
102. Surface Science seminar, Department of Physics, University of Maryland, College Park, MD, May 1996.
103. APS March Meeting, St Louis, MO, March 1996.
104. Surface Science seminar, Departments of Chemical Engineering and Chemistry, University of California, Santa Barbara, CA, December 1995.
105. Surface Science seminar, Sandia National Laboratory, Albuquerque, NM, August 1995.
106. Kamp Chaos, Lake Arrowhead, CA, May 1995.
107. Graduate Student Seminar, Program in Applied Mathematics, University of Colorado, Boulder, CO, February 1995.
108. Minisymposium on Phase Transitions in Catalytic Surface Reaction Models, University of Minnesota, Minneapolis, MN, June 1994.
109. Kamp Chaos, Lake Arrowhead, CA, May 1994.
110. Center for Nonlinear Studies, Los Alamos National Laboratory, May 1994.
111. Nonlinear Dynamics seminar, Applied Mathematics Department, University of New South Wales, Sydney, NSW, Australia, December 1993.
112. Chemical Physics After Dark, University of Colorado, Boulder, CO, November 1993.
113. 6th Annual Copper Mountain Conference on Multigrid Methods, Copper Mountain, CO, April 1993.
114. Los Alamos Days at Boulder, Program in Applied Mathematics, University of Colorado, Boulder, CO, March 1993 (poster).

Recognition of Work in Scientific and Popular Press

1. "Taking the heat off distillation", Chemical & Engineering News June 19, 2017
2. Georgia Tech ChBE seminar "The Secrets of Memorably Bad Presentations" covered by Retraction Watch and Chemical and Engineering News, 2017.
3. April 2016 Comment Article in *Nature* by Sholl and Lively covered by outlets including Scientific American, Phys.org, ChemEurope.com, Chem.info.
4. "Supercomputing has a future in clean energy", *Physics Today*, July 2011, 27-28.
5. "Call for Clean Energy Innovation", *Chemical & Engineering News*, June 13, 2011, 29-31
6. "Risky energy research faces uncertain future", *Nature*, March 10 2011, p. 145-146.
7. "Chemical Processing With One Hand", *Chemical Engineering Progress*, October 2009, p.16.

8. *Phys. Chem. Chem. Phys.* **9** (2007) 1438-1452 featured as an “Editor’s Choice” paper in *Science*, March 23, 2007 and highlighted as a “2007 chemistry breakthrough” in *Chemistry World*, December 18, 2007.
9. “Filling Up On Hydrogen”, *Chemical and Engineering News*, August 22, 2005 (cover story).
10. “Taking The Pulse Of Catalysis Funding”, *Chemical and Engineering News*, November 17, 2003.
11. “Carbon Nanotubes Show Promise as Gas Separation Membranes”, *Chemical Engineering Progress*, December 2002.
12. “Nanotubes Could Reduce CO₂ Emissions”, *United Press International*, September 9, 2002. This story was subsequently reprinted in smalltimes.com, Design News and other online outlets.
13. “Chiral Surface Chemistry”, *Chemical and Engineering News*, March 25, 2002 (cover story).
14. “A Hydrogen Filter From Nanotubes”, *Physical Review Focus*, February 1, 1999.

Other Public Products

1. “The Secrets of Memorably Bad Presentations”, Georgia Tech ChBE seminar, Fall 2016, <https://www.youtube.com/watch?v=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. DOE BES, NEETER Energy Earthshot Research Center, \$19,000,000, 9/23-9/27 (Sholl is PI, co-PIs from Oak Ridge National Laboratory and 5 university partners)
2. Transformational Decarbonization Initiative, Oak Ridge National Laboratory LDRD Program, \$25,000,000, 10/21-9/26 (Sholl is PI)
3. NASA, “Advanced sorbent system for oxygen recovery from helium”, \$37,500, 9/1/20-8/31/21 (subcontract from TDA)
4. ExxonMobil Research and Engineering, “Quantitative Predictions of Molecular Transport in Zeolites”, \$296,000, 10/1/20-10/1/21
5. Sandia National Laboratories, “Smart Materials for Highly Complex Optical Tags with Environmental Response”, \$187,000, 10/1/19-9/30/22
6. ExxonMobil Research and Engineering, “Computational Modeling of Specific Interactions of Non-hydrocarbon species”, \$114,000, 11/1/18-11/1/19
7. 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)
8. Department of Energy Advanced Manufacturing Office, “NNMI/RAPID – Focus Area Leader”, \$200,000, 4/1/17-12/31/20 (subcontract from AIChE)
9. 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)

10. Sandia National Laboratory, “Engineered Materials for Deactivation of Chemical Agents”, \$118,000, 10/1/17-9/30/19
11. ExxonMobil Research and Engineering, “Quantitative Predictions of Diffusion in Zeolites”, \$434,000, 4/16/16-4/15/19
12. ExxonMobil Upstream Research, “Modeling Adsorption of Polar Molecules in Complex Adsorbents”, \$548,000, 10/16/15-10/15/19
13. ExxonMobil Research and Engineering, “Modeling Molecular Transport of Gas and Liquid Mixtures in Microporous Materials”, \$339,000, 9/6/16-9/14/19
14. 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)
15. 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)
16. 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)
17. 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)
18. 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)
19. 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)
20. Oak Ridge National Laboratory, “GO Project: Discovery, Understanding and Validation of Layered Materials”, \$110,000, 5/1/14-4/30/16
21. Oak Ridge National Laboratory, “GO Project: Layered Ferroics”, \$110,000, 9/1/14-8/30/16
22. 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)
23. 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)
24. 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).
25. ExxonMobil Research and Engineering, “Adsorption in Zeolites”, \$820,000, 10/13-10/17
26. 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)

27. 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)
28. Phillips66, “Advanced Materials and Membranes for Gas Separations”, \$900,000, 10-12-9/15 (Nair is PI, Sholl and Jones are co-PIs)
29. ExxonMobil Chemicals, “Recovery of olefins from naphtha using MOFs”, \$342,000, 11/12-10/14 (Sholl is PI, Nair is co-PI)
30. ExxonMobil Chemicals, “Identification of MOFs for xylene enrichment”, \$378,000, 10/12-9/14 (Sholl is PI, Nair is co-PI)
31. Dow Chemical, “Membrane reactors for hydrocarbon processing”, \$2,000,000, 10/10-9/14 (Nair is PI, Jones and Sholl are co-PIs)
32. 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)
33. 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)
34. 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)
35. 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)
36. 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)
37. Sandia National Laboratory, “Computational modeling of nanoporous framework materials”, \$240,000, 3/10-8/13
38. 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)
39. 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
40. 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),
41. 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.
42. 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)
43. Dow Corporation, “Ethanol, Propanol and other high alcohol synthesis from H₂/CO, a combined experimental and computational approach”, \$1,184,000 (C. Jones is PI, Sholl is one of 2 co-PIs), 9/08-8/11
44. ConocoPhillips Corporation, “Advanced Materials and Membranes for Gas Separations”, \$2,376,656 (S. Nair is PI, Sholl is one of 4 co-PIs), 1/09-6/12

45. 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
46. Department of Energy, Office of Basic Energy Sciences, “Ab initio screening of alloys for hydrogen purification membranes”, \$450,000, 8/08-7/11.
47. Georgia Tech Creating Energy Options Program, “Amorphous Metal Alloys for Hydrogen Purification Membranes”, \$38,500, 7/08-6/09
48. National Science Foundation, “The transition state in catalysis: experiment and computational modeling”, \$494,743, 4/07-2/10 (A. Gellman, PI; Sholl co-PI).
49. 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).
50. 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).
51. 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).
52. Pennsylvania Infrastructure Technology Alliance, “Spectroscopic Characteristics of Nanostructured Chiral Surfaces”, \$44,000, 9/06-5/08 (A. Gellman, PI; Sholl co-PI).
53. 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.
54. 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).
55. 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).
56. 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).
57. Department of Energy, Basic Energy Sciences, “Rapid ab initio screening of ternary alloys for hydrogen purification”, \$300,000, 7/05-6/08.
58. Department of Energy, “First principles quantum chemistry approaches to predicting surface segregation in metal alloy hydrogen membranes”, \$50,000, 9/05-8/06.
59. Sandia National Laboratory, “Atomically detailed simulations of molecular mixtures in cationic zeolites”, \$20,000, 5/05-9/05.
60. Merck Company Foundation, “Separation of Chiral Compounds Using Chiral Surfaces”, \$90,000, 8/04-7/07.
61. 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.

62. 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.
63. 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.
64. Sandia National Laboratory, “Atomically-detailed simulations of mixture adsorption in zeolites”, \$30,000, 3/04-9/04.
65. 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).
66. Pennsylvania Infrastructure Technology Alliance, “Computational Thermochemistry of GaAs Contaminants”, \$5,500, 11/03-1/04. (Sholl is PI, D. Yaron is co-PI.)
67. ACS Petroleum Research Fund, “Density Functional Theory and Lattice Gas Models of Hydrogen Diffusion in CuPd Alloys”, \$80,000, 5/03-8/05.
68. National Science Foundation, "Catalysis and Separations With One Hand", \$320,000 (Sholl is PI, A. Gellman is co-PI), 9/02-9/05.
69. 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.
70. ACS Petroleum Research Fund, “Chiral Surfaces Symposium”, \$3,600, 3/03-8/03 (on behalf of the ACS Colloids and Surfaces Division).
71. 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.
72. National Science Foundation, “2002 Midwest Thermodynamics and Statistical Mechanics Meeting, May 13-14, 2002, Pittsburgh, PA”, \$6400, 5/02-5/03.
73. Camille Dreyfus Teacher-Scholar Award, \$60,000, 2002.
74. E. Kears Pollock/PPG Industries Grant for Young Faculty, \$100,000, 2002-2005.
75. 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.)
76. 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.
77. Sloan Foundation Fellowship, \$40,000, 6/01-5/03.
78. 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).
79. 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.)
80. National Energy Technology Laboratory, Department of Energy, “Computational Screening of Zeolites for CO₂ Sequestration”, \$157,402, 3/01-3/03.
81. National Energy Technology Laboratory, Department of Energy, “University/NETL Student Partnership”, \$30,000, 9/00-8/01.

82. 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).
83. Air Products and Chemicals Inc., “Fundamental Studies of Molecular Diffusion in Zeolite Cavities”, \$15,000, 9/00-8/01.
84. Air Products and Chemicals Inc., “Corrosion of Metal Surfaces by Metal Dusting”, \$25,000, 9/00-9/01.
85. National Science Foundation CAREER Award, “Atomically Detailed Modeling of Transport Through Zeolite Membranes”, \$215,000, 4/00-3/04
86. American Chemical Society Petroleum Research Fund, “Microscopic Characterization of Adsorption and Transport in Aluminophosphate Molecular Sieves”, \$20,000, 9/98-8/00.
87. Carnegie Mellon Faculty Development Fund, “Rational Design of Microporous Membranes using Zeolites and Pore-forming Proteins”, \$5,814, 4/98-4/99.
88. National Science Foundation, "Catalysis With One Hand", \$315,000 (Sholl is PI, A. Gellman is co-PI), 6/99-5/02.
89. National Science Foundation, “Morphological Instability in CdTe Homoepitaxy”, \$100,000 (P. Sides is PI, Sholl is co-PI), 7/99-6/00.
90. Carnegie Mellon Interdisciplinary Course Development Fund, "Development of an Interdisciplinary Course on Molecular Simulations, \$7,500, 7/99-5/00.

Professional Activities

Journal editing:

- Editor-in-Chief, *AIChE Journal*, 2021-present
- Senior editor, *Langmuir*, 2009-2019 (~300 manuscripts per year)
- Member of Elsevier Engineering and Technology Advisory Board, 2008-2010
- Member of Editorial Advisory Board, *Langmuir*, 2008-2009
- Guest editor (with A. Gellman) of special issue of *Journal of Molecular Catalysis A: Chemical* titled “Heterogeneous Chiral Catalysis” Vol. 228 Issues 1-2, 2005
- Guest editor of special issue of *Catalysis Today* titled “Modeling of Catalysis”, Vol. 105, Issue 1, 2005.

Professional Societies:

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

Advisory Boards:

- Department of Chemical Engineering, University of Texas, Austin (2013-2016)
- Department of Chemical Engineering, The Pennsylvania State University, State College, PA (2014-1019)
- Department of Chemical & Biological Engineering, Johns Hopkins University, Baltimore, MD (2016-present)

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

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

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

Conference Organization:

Chair, Gordon Conference on Chemical Separations, 2020
Organizing Committee, Chemical Engineering National Diversity Equity Workshop, 2021
Co-chair (with S. Nair), International Conference on Inorganic Membranes, 2016
Chair, Gordon Conference on Nanoporous Materials, August 2015
Vice-Chair, Gordon Conference on Nanoporous Materials, August 2013
Co-organizer (with J. K. Johnson), 2002 Midwest Thermodynamics and Statistical Mechanics Meeting

Conference Sessions Chaired:

Session Chair, Process Intensification Topical Conference, AIChE Spring Meeting, San Antonio, TX (6 sessions of invited talks)
Symposium co-chair, "Hydrogen Storage and Purification", AIChE Annual Meeting, Salt Lake City, UT, November 2010
Symposium co-chair, "Chiral Surfaces", ACS National Meeting, Boston, MA, August 2010
Symposium co-chair, "Computational Materials Design in Chemical Industries", ACS National Meeting, San Francisco, California, September 10-14, 2006
Symposium co-chair, "Chirality and Enantioselectivity at Surfaces", ACS National Meeting, San Francisco, California, September 10-14, 2006
Symposium Chair, "Chiral Surfaces", ACS National Meeting, New Orleans, LA, March 2003.
Session vice chair, "Diffusion in Microporous Materials I" and "Diffusion in Microporous Materials II", 2003 AIChE Annual Meeting

Session vice chair, “Thermodynamics and Transport Properties (Posters)”, 2003 AIChE Annual Meeting
Organizing committee member, “2003 International Workshop on Zeolitic and Microporous Membranes
Symposium chair, “Computational Methods for Fuels Science”, Fuels Division, 2002 ACS National Meeting
Nottingham Competition Judge, 62nd Physical Electronics Conference, Atlanta, GA, June 2002.
Session vice-chair, “Theory and Simulation on the Mesoscale”, 2001 AIChE National Meeting
Session vice-chair, “Fundamentals of Surface Processes”, 2001 AIChE National Meeting
Symposium co-organizer, “Simulation and Theory of Surfaces, Interfaces, and Complex Fluids”, 2001 ACS Colloids and Surface Science Symposium
Executive committee member, 2001 ACS Colloids and Surface Science Symposium
Session vice-chair, “Theory and Simulation on the Mesoscale”, 2000 AIChE National Meeting
Session presider, “Physical Chemistry of Chirality”, 2000 ACS National Meeting
Session vice-chair, “New Approaches for Simulating Long Time Phenomena”, 1999 AIChE National Meeting

Government Committees

External reviewer, National Academies Study Committee, Carbon Utilization Infrastructure, Markets and Research and Development, 2024
Panel member, National Academies Study Committee, Chemical Engineering: Challenges and Opportunities in the 21st 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 CO₂ Capture and Sequestration, Tulane University, New Orleans, LA, March 2002 – invited participant

Departmental and University Committees

Departmental Computing Committee (CMU) (1999-2000. Chair 2001,2002)
Department PhD Qualifying Exam Committee (CMU) (1999-2002. Chair 2002. 2006)
Department Graduate Recruiting Committee (CMU) (Chair, 2002-2005)

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

PhD Committees

Committee member on > 70 PhD theses since 2000.

Ph.D. Graduate Students Supervised

1. Timothy D. Power (Graduated 12/01. Postgraduation employer: Shell)
2. Anastasios Skoulidas (Graduated 5/03. Current employer: Exxon Mobil)
3. Aravind Asthagiri (Graduated 5/2003. Current employer: Associate Professor, Ohio State University)
4. Preeti Kamakoti (Graduated 5/05. Postgraduation employer: ExxonMobil)
5. Chong Shang-Shan [Department of Physics] (Graduated 6/05)
6. Rees Rankin (Graduated 5/06. Postgraduation employer: University of Pittsburgh)
7. David Newsome (Graduated 5/06. Postgraduation employer: TUDelft)
8. Bhawna Bhatia (Graduated 9/06. Postgraduation employer: Intel)
9. Haibin Chen (Graduated 8/07. Postgraduation employer: Carbozyme)
10. Xin Li [Department of Chemistry] (Graduated 1/07)
11. Sudhakar Alapati (Graduated 8/07. Postgraduation employer: Intel)
12. Joanna James (Graduated 7/2008. Postgraduation employer: Air Products and Chemicals)
13. Lymarie Semidey-Flecha (Graduated 7/2009. Postgraduation employer: ORNL)
14. Chen Ling (Graduated 12/2009. Postgraduation employer: University of Michigan)
15. Seda Keskin (Graduated 12/2009. Postgraduation employer: Koc University)
16. Sang Eun Jee (Graduated 5/2010. Postgraduation employer: Carnegie Mellon University)
17. Jeong Woo Han (Graduated 5/2010. Postgraduation employer: MIT)
18. Ki Chul Kim (Graduated 8/2010. Postgraduation employer: Northwestern University)
19. Mohamad Kassae [co-advised with Sankar Nair] (Graduated 8/2012. Postgraduation employer: Georgia Tech)
20. Emmanuel Haldoupis (Graduated 5/2013. Postgraduation employer: University of Minnesota)
21. Sung Gu Kang (Graduated 5/2013. Postgraduation employer: Cornell University)
22. Liwei Li (Graduated 5/2014. Postgraduation employer: Dow Chemical Company)
23. Nita Chandrasekhar (Graduated 5/2014. Postgraduation employer: Praxair)
24. Dieh Teng (Graduated 5/2014. Postgraduation employer: KBR)

25. Ambarish Kulkarni (Graduated: 12/2014. Postgraduation employer: Stanford University)
26. Kelly Nicholson (Graduated 8/2014. Postgraduation employer: Praxair)
27. Daniel Wei (Graduated 12/2014)
28. Jason Gee (Graduated 8/2015. Postgraduation employer: ExxonMobil)
29. Ben Chun [co-advised with Seung Sung Jang] (Graduated 5/2015)
30. Rohan Awati (Graduated 12/2015) [Georgia Tech]
31. Hakan Demir (Graduated 5/2016) [University of Minnesota]
32. Seung Won Choi [co-advised with Sankar Nair and Chris Jones] (Graduated 5/2016) [LG Chemicals]
33. Jeffrey Camp (Graduated 5/2016) [LLBL]
34. Ross Verploegh (Graduated 8/2017) [GT]
35. Dalar Nazarian (Graduated 8/2016) [Praxair]
36. Lalit Darunte [co-advised with Krista Walton and Chris Jones] (Graduated 5/2018) [Dow Chemicals]
37. Jungseob So [co-advised with Carsten Sievers] (Graduated 5/2018) [Samsung]
38. Yang Liu (Graduated 12/2018) [Dow Chemical]
39. Chu Han (Graduated 12/2018)
40. Souryadeep Bhattacharyya [co-advised with Sankar Nair] (Graduated 12/2018) [GT]
41. Rebecca Han (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. Yuhan Yang (Graduated 8/2022) [Harbin University]
48. Ifayoyinsola (Yoyin) Ibikunle (Graduated 5/2023)
49. Zhenzi Yu (Graduated 8/2023) [Boehringer Ingelheim]
50. Alan Daou (Graduated 5/2024)
51. Arvind Ganesan [co-advised with Sankar Nair] (Graduated 8/2023) [ORNL]
52. Xuqing Cai (Graduated 12/2023)
53. Chao-Wen Chang (expected graduation: 12/2024)
54. Shubham Jamdade (expected graduation: 12/2024)
55. Xiaohan Yu (expected graduation: 12/2024)
56. Brandon Bout [co-advised with Krista Walton] (Graduated 5/2024)
57. Akriti Sarswat [co-advised with Ryan Lively] (expected graduation: 5/2025)
58. Jia Yuan Chng (expected graduation: 5/2025)
59. Logan Brabson (expected graduation: 5/2025) [co-advised with AJ Medford]
60. Surbhi Kumar (expected graduation: 12/2025) [co-advised with Krista Walton]

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-present (formally reporting to Prof. Ryan Lively since 7/21)
12. Dr. Iyad Hijazi, 1/11-1/12
13. Dr. Salah Boulfefel, 6/12-present (formally reporting to Prof. Ryan Lively since 7/21)
14. Dr. Veronika Walkosz, 8/12-9/13
15. Dr. Rongshun Zhu, 9/12-10/14
16. Dr. Melissa Lucero, 11/12-3/14
17. Dr. Xiaowa Nie, 8/14-1/15

18. Dr. Joshua Howe, 11/14-7/18
19. Dr. Dai Tang, 1/16-3/22
20. Dr. Rohan Awati, 9/16-10/18
21. Dr. Alex Hyla, 1/17-12/17
22. Dr. Anh Pham, 1/18-5/18
23. Dr. Farhad Gharagheizi, 6/18-11/22
24. Dr. Raghuram Thyagarajan, 8/18-10/23
25. Dr. Jifeng Sun, 11/18-2/23