CURRICULUM VITAE

Brian Space, PhD
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Statement of Professional Philosophy

My skills as an investigator, advisor and instructor are complementary. The focus is always to learn, communicate and grow. I seek to be a mentor in the classroom and laboratory, to share the fascination and joy I have in exploring the nature of the universe. I explain to students that science was mislabeled as a noun in English; it is the active pursuit of knowledge that has made science and engineering indispensable to humanity. The few yet profound things we have discovered in the past few centuries are just the beginning if we effectively train and motivate the next generation of scientific explorers.

My greatest passion is working with other researchers and especially student investigators. I maintain a positive, close and productive relationship with my diverse group of current and former graduate students and several undergraduates. My strengths include mentoring and building a community of learning and exploration. If my students can flourish, I will too. This commitment continues in my desire to build a better department and university, while serving my profession and community. I am looking for an opportunity to further facilitate these aspirations.

To establish expectations for my professional interactions, I have established a mission statement for my research group that leads our web page http://chemistry.usf.edu/faculty/space/

The Space Group mission is: 1) to foster qualitative and quantitative reasoning skills individually and through our interactions with others; 2) to develop informed writing, speaking and presentation skills; 3) to perform and facilitate world class science with integrity, discipline and high ethical standards; and 4) to seek new knowledge, going boldly where no one has gone before. In pursuit of this mission we seek to serve our university, community, society, the world and universe. Our goal is balanced, sustainable progress on the elements of our mission.

Personal Attributes

Dedicated educator with over 20 years of teaching experience in the chemistry discipline.

Vast expertise in fundamental and practical computational studies in materials modeling with an emphasis on energy / environment related applications.

Respected professional committed to excellence in research, teaching, mentoring and collaboration.

Ability to excel in a demanding, outcome-oriented, and dynamic work environment.

Utilize innovative teaching strategies that challenge students and promote their success.

Skilled in conceving and conducting research, grant writing, and academic project management.

Experience as foundational departmental faculty member at a Research I university.

Professional level strategist, poker player and author.

Formal Education

PhD, Chemistry 1992
Boston University, Boston, MA

Developed novel computer simulation methods for mixed quantum-classical dynamics.

Characterized excess electronic relaxation processes in liquids.

Studied the nature of conducting electronic states in fluids.

Co-Organized and created the “Manhattan Poster Project” between B.U., M.I.T, Columbia and Yale universities. A graduate student sponsored rotating meeting with student presenters and faculty participants that continued for over a decade.

BA, Chemistry 1988
Boston University, Boston, MA

Performed undergraduate research in molecular biology at M.I.T. with Paul Schimmel.

Made site-directed mutant of alanin tRNA synthetase.

Performed undergraduate research in experimental physical chemistry at B.U. with Erwin Poliakoff.

Published research on modeling photoionization and experimental synchrotron experiments.

Faculty Experience

University of South Florida **Overall 2000 - Present**
Tampa, FL

Professor, Department of Chemistry 2012 – Present
Professor and Associate Chair, Department of Chemistry 2010 – 2012
Associate Professor, Department of Chemistry 2000 – 2006

Established an internationally recognized research program with metrics reflecting our accomplishments (google scholar 10/2018):

Citation indices	All	Since 2013
Citations	4529	3268
h-index	35	28
i10-index	81	61

Built a sustainable research group that emphasis graduate and undergraduate training.

Built an effective teaching program that stresses interactive classrooms and critical thinking.

Worked to build a nationally ranked chemistry department.

Created and implemented a modern graduate doctoral program in chemistry.

Served the university and community to make an impact beyond my discipline.

Courses Taught:

Physical Chemistry I & II

General Chemistry I & II

Quantum Mechanics I & II

Statistical Mechanics I & II

Historical Perspectives in Chemistry

Methods I & II

Special Topics in Computational Chemistry

Assistant Professor, Department of Chemistry 1995 – 2000
Duquesne University, Pittsburgh, PA

Research Associate 1992 – 1995
Princeton University, Princeton, NJ

Developed molecular dynamics simulation methods for study of proteins and condensed phase systems.

Theoretical modeling of the long time dynamical behavior of proteins and polymers funded by NSF CISE postdoctoral fellowship.

Articles, Research and Presentations

(***Bold & Italics*** authors are Space group graduate students and *italics only* are undergraduates)

Featured Papers

Porous materials with optimal adsorption thermodynamics and kinetics for CO_2 separations. Nugent, P.; Belmabkhout, Y.; Burd, S. D.; Cairns, A. J.; Luebke, R.; ***Forrest, K. A.; Pham***, ***T.***; Ma, S.; Space, B.; Wojtas, L.; Eddaoudi, M.; Zaworotko, M. J. Nature. 2013, 495, 80-84.

On the Mechanism of Hydrogen Storage in a Metal-Organic Framework Material. ***Belof, J. L.; Stern, A. C.***; Eddaoudi, M.; Space, B., J. Am. Chem. Soc. 2007, 129 (49), 15202-15210.

Introduction of π-Complexation into Porous Aromatic Framework for Highly Selective Adsorption of Ethylene over Ethane. Li, B.; Zhang, Y.; Krishna, R.; Yao, K.; Han, Y.; Wu, Z.; Ma, D.; Shi, Z.; ***Pham, T.***; Space, B.; Liu, J.; Thallapally, P. K.; Liu, J.; Chrzanowski, M.; Ma, S. J. Am. Chem. Soc. 2014, 136 (24), 8654-8660.

Theoretical modeling of interface specific vibrational spectroscopy: methods and applications to aqueous interfaces. ***Perry, A.; Neipert, C.***; Space, B.; Moore, P. B., Chem Rev 2006, 106 (4), 1234-58.

A Robust Molecular Porous Material with High CO_2 Uptake and Selectivity. Nugent, P.S.; Rhodus, V.L.; ***Pham, T.; Forrest, K.***; Wojtas, L.; Space, B.; Zaworotko, M.J. J. Am. Chem. Soc., 2013, 135 (30), 10950–10953.

Identification of a wagging vibrational mode of water molecules at the water/vapor interface. ***Perry, A.; Neipert, C.; Ridley, C.***; Space, B.; Moore, P. B., Physical Review E 2005, 71 (5), 050601.
The predicted vibrational Wagging Mode was measured experimentally a decade later with the shape and location predicted!

Papers with Current Students

Hydrogen Adsorption in a Zeolitic Imidazolate Framework with lta Topology. ***Pham, T.; Forrest, K. A.***; Furukawa, H.; Eckert, J.; Space, B..J. Phys. Chem. C 2018, 122 (27), 15435–15445.

Robust Ultramicroporous Metal–Organic Frameworks with Benchmark Affinity for Acetylene. Peng, Y.; ***Pham, T.***; Li, P.; Wang, T.; Chen, Y.; Chen, K.-J.; ***Forrest, K. A.***; Space, B.; Cheng, P.; Zaworotko, M. J.; Zhang, Z..Angew. Chem. Int. Ed. 2018, 57 (34), 10971–10975

Investigating C_2H_2 Sorption in a–$[M_3(O_2CH)_6]$ (M = Mg, Mn) Through Theoretical Studies. ***Forrest, K. A.; Franz, D. M.; Pham, T.***; Space, B. Cryst. Growth Des. 2018, 18 (9), 5342 - 5352.

Readily accessible shape-memory effect in a porous interpenetrated coordination network. Shivanna, M.; Yang, Q.-Y.; Bajpai, A.; Sen, S.; Hosono, N.; Kusaka, S.; ***Pham, T.; Forrest, K. A.***; Space, B.; Kitagawa, S.; Zaworotko, M. J. Sci. Adv. 2018, DOI: DOI: 10.1126/sciadv.aaq1636.

Theoretical study of the effect of halogen substitution in molecular porous materials for CO_2 and C_2H_2 sorption. ***Franz, D. M.;*** *Djulbegovic, M.****; Pham, T.***; Space, B. AIMS Mater. Sci. 2018, 5 (2), 226–245.

Impact of partial interpenetration in a hybrid ultramicroporous material on C_2H_2/C_2H_4 separation performance. O'Nolan, D.; Madden, D. G.; Kumar, A.; Chen, K.-J.; ***Pham, T.; Forrest, K. A.***; Patyk-Kazmierczak, E.; Yang, Q.-Y.; Murray, C. A.; Tang, C. C.; Space, B.; Zaworotko, M. J. Chem. Commun. 2018, 54 (28), 3488–3491.

Efficient CO_2 Removal for Ultra-Pure CO Production by Two Hybrid Ultramicroporous Materials. Chen, K.-J.; Yang, Q.-Y.; Sen, S.; Madden, D. G.; Kumar, A.; ***Pham, T.; Forrest, K. A.***; Hosono, N.; Space, B.; Kitagawa, S.; Zaworotko, M. J. Angew. Chem. Int. Ed. 2018, 57 (13), 3332–3336.

A Stable Metal–Organic Framework Featuring Local Buffer Environment for Carbon Dioxide Fixation He, H.; Sun, Q.; Gao, W.; Perman, J. A.; Sun, F.; Zhu, G.; Aguila, B.; ***Forrest, K.***; Space, B.; Ma, S..Angew. Chem. Int. Ed. 2018, 57 (17), 4657–4662.

Simulations of hydrogen, carbon dioxide, and small hydrocarbon sorption in a nitrogen-rich rht-metal–organic framework. ***Franz, D.;*** *Dyott, Z.****; Forrest, K.; Hogan, A.; Pham, T.***; Space, B. Phys. Chem. Chem. Phys. 2018, 20, 1761 - 1777. DOI: 10.1039/c7cp06885a.

Investigating gas sorption in an rht-metal–organic framework with 1,2,3-triazole groups. ***Forrest, K. A.; Pham, T.***; Space, B. Phys. Chem. Chem. Phys. 2017, 19, 29204 - 29221.

The effect of centered versus offset interpenetration on C_2H_2 sorption in hybrid ultramicroporous materials. Bajpai, A.; O'Nolan, D.; Madden, D. G.; Chen, K.-J.; ***Pham, T.***; Kumar, A.; Lusi, M.; Perry IV, J. J.; Space, B.; Zaworotko, M. J. Chem. Commun., 2017 53 (84), 11592–11595, DOI: 10.1039/C7CC05882A.

Experimental and Theoretical Investigations of the Gas Adsorption Sites in rht-Metal–Organic Frameworks. ***Pham, T.; Forrest, K. A.; Franz, D.***; Space, B. CrystEngComm, 2017, 19 (32), 4646–4665.

Comparing the mechanism and energetics of CO_2 sorption in the SIFSIX series. ***Forrest, K. A.; Pham, T.***; Space, B. CrystEngComm, 2017, 19 (24), 3338–3347.

Predictive models of gas sorption in a metal–organic framework with open-metal sites and small pore sizes. ***Pham, T.; Forrest, K. A.; Franz***, D. M.; Guo, Z.; Chen, B.; Space, B. Phys. Chem. Chem. Phys., 2017, 19 (28), 18587–18602.

The rotational dynamics of H_2 adsorbed in covalent organic frameworks. ***Pham, T.; Forrest, K. A.;*** *Mostrom, M.*; Hunt, J. R.; Furukawa, H.; Eckert, J.; Space, B. Phys. Chem. Chem. Phys. 2017, 19 (20), 13075–13082.

Fine Tuning of MOF-505 Analogues to Reduce Low Pressure Methane Uptake and Enhance Methane Working Capacity. Zhang, M.; Zhou, W.; ***Pham, T.; Forrest, K. A.***; Liu, W.; He, Y.; Wu, H.; Yildirim, T.; Chen, B.; Space, B.; Pan, Y.; Zaworotko, M. J.; Bai, J. Angew. Chem. Int. Ed. 2017, DOI: 10.1002/anie.201704974.

Highly selective separation of C_2H_2 from CO_2 by a new dichromate-based Hybrid Ultramicroporous Material. Scott, H. S.; Shivanna, M.; Bajpai, A.; Madden, D.; Chen, K.-J.; ***Pham, T.; Forrest, K.; Hogan, A.***; Space, B.; Perry IV, J.; Zaworotko, M. ACS Appl. Mater. Interfaces 2017, 9 (39), 33395-33400.

High H_2 Sorption Energetics in Zeolitic Imidazolate Frameworks. ***Pham, T.; Forrest, K. A.***; Furukawa, H.; Russina, M.; Albinati, A.; Georgiev, P. A.; Eckert, J.; Space, B. J. Phys. Chem. C 2017, 121 (3), 1723–1733. DOI: 10.1021/acs.jpcc.6b1146

Effect of ring rotation upon gas adsorption in SIFSIX-3-M (M = Fe, Ni) pillared square grid networks. Elsaidi, S. K.; Mohamed, M. H.; Simon, C. M.; Braun, E.; ***Pham, T.; Forrest, K. A.***; Xu, W.; Banerjee, D.; Space, B.; Zaworotko, M. J.; Thallapally, P. K. Chem. Sci. 8(3) 2373-2380 2017. DOI: 10.1039/C6SC05012C

Benchmark C_2H_2/CO_2 and CO_2/C_2H_2 Separation by Two Closely Related Hybrid Ultramicroporous Materials. Chen, K.-J.; Scott, H. S.; Madden, D. G.; ***Pham, T.***; Kumar, A.; Bajpai, A.; Lusi, M.; ***Forrest, K. A.***; Space, B.; Perry IV, J. J.; Zaworotko, M. J. Chem 2016, 1(5), 753–765. DOI: http://dx.doi.org/10.1016/j.chempr.2016.10.009

Towards an understanding of the propensity for crystalline hydrate formation by molecular compounds. Bajpai, A.; Scott, H. S.; ***Pham, T.***; Chen, K.-J.; Space, B.; Lusi, M.; Perry, M. L.; Zaworotko, M. J. IUCrJ 2016, 3 (6), 430-439. DOI: 10.1107/S2052252516015633.

Theoretical Investigations of CO_2 and H_2 Sorption in Robust Molecular Porous Materials. ***Pham, T.; Forrest, K. A.***; Chen, K.-J.; Kumar, A.; Zaworotko, M. J.; Space, B.Langmuir 2016 32(44), 11492-11505. DOI: 10.1021/acs.langmuir.6b03161

Accurate H_2 Sorption Modeling in the rht-MOF NOTT-112 Using Explicit Polarization. ***Franz, D.; Forrest, K. A.; Pham, T.***; Space, B. Cryst. Growth Des. 2016, DOI: 10.1021/acs.cgd.6b01058.

Tuning Pore Size in Square-Lattice Networks for Size-Selective Sieving of CO_2. Chen, K.-J.; Madden, D. G.; ***Pham, T.; Forrest, K. A.***; Kumar, A.; Yang, Q.-Y.; Xue, W.; Space, B.; Perry IV, J. J.; Zhang, J.-P.; Chen, X.-M.; Zaworotko, M. J. Angew. Chem. Int. Ed. 2016, 55 (35), 10268–10272.

An unusual H_2 sorption mechanism in PCN-14: insights from molecular simulation. ***Pham, T.; Forrest, K. A.***; Space, B. Phys. Chem. Chem. Phys. 2016, 18, 21421 - 21430

Dynamics of H_2 adsorbed in porous materials as revealed by computational analysis of inelastic neutron scattering spectra. ***Pham, T.; Forrest, K. A.***; Space, B.; Eckert, J. Phys. Chem. Chem. Phys. 2016, 18, 17141–17158.

Hybrid Ultra-Microporous Materials for Selective Xe Adsorption and Separation. Mohamed, M. H.; Elsaidi, S. K.; ***Pham, T.; Forrest, K. A.***; Schaef, H. T.; ***Hogan, A.***; Wojtas, L.; Xu, W.; Space, B.; Zaworotko, M. J.; Thallapally, P. K. Angew. Chem. Int. Ed. 2016, 55 (29), 8285–8289. .

Crystal engineering of a family of hybrid ultramicroporous materials based upon interpenetration and dichromate linkers. Scott, H. S.; Ogiwara, N.; Chen, K.-J.; Madden, D. G.; ***Pham, T.; Forrest, K.***; Space, B.; Horike, S.; Perry IV, J. J.; Kitagawa, S.; Zaworotko, M. J. Chem. Sci. 2016, 7, 5470–5476.

Exceptional H_2 sorption characteristics in a Mg^{2+}-based metal–organic framework with small pores: insights from experimental and theoretical studies. ***Pham, T.; Forrest, K. A.***; Falcão, E. H. L.; Eckert, J.; Space, B. Phys. Chem. Chem. Phys. 2016, 18(3), 1786–1796.

Dramatic Effect of the Electrostatic Parameters on H_2 Sorption in an M-MOF-74 Analogue. ***Pham, T.; Forrest, K. A.***; Eckert, J.; Space, B. Cryst. Growth Des. 2016, 16(2), 867–874.

Crystal Engineering of a 4,6-c fsc Platform That Can Serve as a Carbon Dioxide Single-Molecule Trap. Elsaidi, S. K.; Mohamed, M. H.; ***Pham, T.***; Hussein, T.; Wojtas, L.; Zaworotko, M. J.; Space, B. Cryst. Growth Des. 2016, 16(2), 1071–1080.

Inelastic Neutron Scattering and Theoretical Studies of H_2 Sorption in a Dy(III)-Based Phosphine Coordination Material. ***Forrest, K. A.; Pham, T.***; Georgiev, P. A.; Embs, J. P.; Waggoner, N. W.; Hogan, A.; Humphrey, S. M.; Eckert, J.; Space, B.Chem. Mater. 2015, 27, 7619–7626.

Correction: Hydrophobic pillared square grids for selective removal of CO_2 from simulated flue gas. Elsaidi, S. K.; Mohamed, M. H.; Schaef, H. T.; Kumar, A.; Lusi, M.; ***Pham, T.; Forrest, K. A.***; Space, B.; Xu, W.; Halder, G. J.; Liu, J.; Zaworotko, M. J.; Thallapally, P. K. Chem. Commun. 2015, 51 16872–16872.

Theoretical Insights into the Tuning of Metal Binding Sites of Paddlewheels in rht-Metal–Organic Frameworks. ***Pham, T.; Forrest, K. A.***; Gao, W.-Y.; Ma, S.; Space, B. ChemPhysChem 2015, 16(15), 3170–3179.

Hydrophobic pillared square grids for selective removal of CO_2 from simulated flue gas. Elsaidi, S. K.; Mohamed, M. H.; Schaef, H. T.; Kumar, A.; Lusi, M.; ***Pham, T.; Forrest, K. A.***; Space, B.; Xu, W.; Halder, G. J.; Liu, J.; Zaworotko, M. J.; Thallapally, P. K. Chem. Commun. 2015, 51, 15530-15533.

Novel mode of 2-fold interpenetration observed in a primitive cubic network of formula $[Ni(1,2\text{-bis}(4\text{-pyridyl})acetylene)_2(Cr_2O_7)]_n$. Scott, H. S.; Bajpai, A.; Chen, K.-J.; ***Pham, T***; Space, B; Perry, J. J.; Zaworotko, M. J. Chem. Commun. 2015, 51, 14832-14835.

Investigating H_2 Sorption in a Fluorinated Metal–Organic Framework with Small Pores Through Molecular Simulation and Inelastic Neutron Scattering. ***Forrest, K. A.; Pham, T.***; Georgiev, P. A.; Pinzan, F.; ***Cioce, C. R.***; Unruh, T.; Eckert, J.; Space, B. Langmuir 2015, 31, 7328-7336.

The local electric field favours more than exposed nitrogen atoms on CO_2 capture: a case study on the rht-type MOF platform. Gao, W.-Y.; ***Pham, T.; Forrest, K. A.***; Space, B.; Wojtas, L.; Chen, Y.-S.; Ma, S. Chem. Commun. 2015, 51, 9636-9639.

Understanding Hydrogen Sorption in In-soc-MOF: A Charged Metal-Organic Framework with Open-Metal Sites, Narrow Channels, and Counterions. ***Pham, T.; Forrest, K. A.; Hogan, A.; Tudor, B.; McLaughlin, K.; Belof, J. L.***; Eckert, J.; Space, B. Cryst. Growth Des. 2015, 15, 1460-1471.

Highly selective adsorption of ethylene over ethane in a MOF featuring the combination of open metal site and π-complexation. Zhang, Y.; Li, B.; Krishna, R.; Wu, Z.; Ma, D.; Shi, Z.; ***Pham, T.; Forrest, K.***; Space, B.; Ma, S. Chem. Commun. 2015, 51, 2714–2717.

Remote Stabilization of Copper Paddlewheel Based Molecular Building Blocks in Metal–Organic Frameworks. Gao, W.; Cai, R.; ***Pham, T.; Forrest, K.; Hogan, A.***; Nugent, P.; Williams, K.; Wojtas, L.; Luebke, R.; Weselinski, L; Zaworotko, M.; Space, B.; Chen, Y; Eddaoudi, M; Shi, X.; Ma, S
Chem. Mater. 2015, 27 (6), pp 2144–2151.

Understanding the H_2 Sorption Trends in the M-MOF-74 Series (M = Mg, Ni, Co, Zn). ***Pham, T.; Forrest, K.A.***; Banerjee, R.; Orcajo, G.; Eckert, J.; Space, B. J. Phys. Chem. C 2015, 119 (2), pp 1078–1090.

Time Correlation Function Modeling of Third-Order Sum Frequency Vibrational Spectroscopy of a Charged Surface/Water Interface. ***Green, A.J.***; Space, B. J. Phys. Chem. B. 2015, 119, 9219–9224.

Modeling PCN-61 and PCN-66: Isostructural rht-Metal–Organic Frameworks with Distinct CO_2 Sorption Mechanisms. ***Pham, T.; Forrest, K. A.;*** *McDonald, K.*; Space, B. Cryst. Growth Des. 2014, 14, 5599–5607.

Capturing the H_2–Metal Interaction in Mg-MOF-74 Using Classical Polarization. ***Pham, T.; Forrest, K. A.; McLaughlin, K.***; Eckert, J.; Space, B. J. Phys. Chem. C 2014, 118, 22683–22690.

A high rotational barrier for physisorbed hydrogen in an fcu-metal–organic framework. ***Pham, T.; Forrest, K.A.***; Georgiev, P.; Lohstroh, W.; Xue, D.-X.; *Hogan, A.*; Eddaoudi, M.; Space, B.; Eckert, J. Chem. Commun. 2014, 50, 14109-14112.

Dramatic effect of pore size reduction on the dynamics of hydrogen adsorbed in metal–organic materials. Nugent, P.; ***Pham, T.; McLaughlin, K.***; Georgiev, P.; Lohstroh, W.; Embs, J. P.; Zaworotko, M. J.; Space, B.; Eckert, J. J. Mater. Chem. A 2014, 2, 13884-13891.

Introduction of π-Complexation into Porous Aromatic Framework for Highly Selective Adsorption of Ethylene over Ethane. Li, B.; Zhang, Y.; Krishna, R.; Yao, K.; Han, Y.; Wu, Z.; Ma, D.; Shi, Z.; ***Pham, T.***; Space, B.; Liu, J.; Thallapally, P. K.; Liu, J.; Chrzanowski, M.; Ma, S. J. Am. Chem. Soc. 2014, 136 (24), 8654-8660.

Insights into an intriguing gas sorption mechanism in a polar metal–organic framework with open-metal sites and narrow channels. ***Forrest, K. A.; Pham, T.; McLaughlin, K.;*** *Hogan, A.*; Space, B. Chem. Commun. 2014, 50, 7283-7286.

Theoretical Investigations of CO_2 and CH_4 Sorption in an Interpenetrated Diamondoid Metal–Organic Material. Pham, ***T.; Forrest, K. A.; Tudor, B.***; Elsaidi, S. K.; Mohamed, M. H.; ***McLaughlin K.; Cioce, C. R.***; Zaworotko, M. J.; Space, B. Langmuir 2014, 30(22), 6454–6462.

Putting the Squeeze on CH_4 and CO_2 through Control over Interpenetration in Diamondoid Nets. Elsaidi, S. K.; Mohamed, M. H.; Wojtas, L.; Chanthapally, A.; ***Pham, T.***; Space, B.; Vittal, J. J. Zaworotko, M. J. J. Am. Chem. Soc. 2014, 136, 5072–5077.

Simulations of Hydrogen Sorption in rht-MOF-1: Identifying the Binding Sites Through Explicit Polarization and Quantum Rotation Calculations. ***Pham, T.; Forrest, K. A.;*** *Hogan, A.****; McLaughlin, K.; Belof, J. L.***; Eckert, J.; Space, B.J. Mater. Chem A 2014, 2, 2088–2100.

Investigating the Gas Sorption Mechanism in an rht-Metal–Organic Framework Through Computational Studies. ***Pham, T.; Forrest, K. A.***; Eckert, J.; Georgiev, P. A.; ***Mullen, A.***; Luebke, R.; Cairns, A. J.; Belmabkhout, Y.; Eubank, J. F.; ***McLaughlin, K.***; Lohstroh, W.; Eddaoudi, M.; Space, B. J. Phys. Chem. C 2014, 118, 439–456.

Efficient calculation of many-body induced electrostatics in molecular systems. ***McLaughlin, K.; Cioce, C. R.; Pham, T.; Belof, J. L.***; Space, B. J. Chem. Phys. 2013, 139, 184112.

A Polarizable and Transferable PHAST N_2 Potential For Use in Materials Simulation. ***Cioce, C. R.; McLaughlin, K.; Belof, J. L.***; Space B.J. Chem. Theory Comput. 2013, 9, 5550–5557.

A Polarizable and Transferable PHAST CO_2 Potential For Materials Simulation. ***Mullen, A. L.; Pham, T.; Forrest, K. A.; Cioce, C. R.; McLaughlin, K.***; Space, B. J. Chem. Theory Comput. 2013, 9, 5421–5429.

Solving the Many-Body Polarization Problem on GPUs: Application to MOFs. ***Tudor, B.***; Space, B. J. Comput. Sci. Ed. 2013, 4, 30–34.

Pillar substitution modulates CO_2 affinity in “mmo” topology networks. Mohamed, M.H.; Elsaidi, S.K.; ***Pham, T.; Forrest, K.A.; Tudor, B.***; Wojtas, L.; Space, B.; Zaworotko, M.J. Chem. Commun., 2013, 49, 9809–9811.

Examining the Effects of Different Ring Configurations and Equatorial Fluorine Atom Positions on CO_2 Sorption in $[Cu(bpy)_2SiF_6]$. ***Forrest, K.A.; Pham, T.***; Nugent, P.; Burd, S.D.; ***Mullen, A.***; Wojtas, L.; Zaworotko, M.J.; Space, B. Cryst. Growth Des., 2013, 13 (10), 4542–4548.

Computational Studies of CO_2 Sorption and Separation in an Ultramicroporous Metal–Organic Material ***Forrest, K.A.; Pham, T.;*** *Hogan, A.****; McLaughlin, K.; Tudor, B.***; Nugent, P.; Burd, S.D.; Mullen, A.; Cioce, C.R.; Wojtas, L.; Zaworotko, M.J.; Space, B. J. Phys. Chem. C, 2013, 117 (34), 17687–17698.

A Robust Molecular Porous Material with High CO_2 Uptake and Selectivity. Nugent, P.S.; Rhodus, V.L.; ***Pham, T.; Forrest, K.***; Wojtas, L.; Space, B.; Zaworotko, M.J. J. Am. Chem. Soc., 2013, 135 (30), 10950–10953.

Understanding Hydrogen Sorption in a Metal–Organic Framework with Open Metal Sites and Amide Functional Groups. ***Pham, T.; Forrest, K. A.***; Nugent, P.; Belmabkhout, Y.; Luebke, R.; Eddaoudi, M.; Zaworotko, M. J.; Space, B. J. Phys. Chem. C, 2013, 117 (18), 9340–9354.

Theoretical Investigations of CO_2 and H_2 Sorption in an Interpenetrated Square-Pillared Metal–Organic Material. ***Pham, T.; Forrest, K.; McLaughlin, K.; Tudor, B.***; Nugent, P.; *Hogan, A.****; Mullen, A.;*** *Cioce, C.R.*; Zaworotko, M.J.; Space, B. J. Phys. Chem. C, 2013, 117 (19), 9970–9982.

Porous materials with optimal adsorption thermodynamics and kinetics for CO_2 separations. Nugent, P.; Belmabkhout, Y.; Burd, S. D.; Cairns, A. J.; Luebke, R.; ***Forrest, K. A.; Pham, T.***; Ma, S.; Space, B.; Wojtas, L.; Eddaoudi, M.; Zaworotko, M. J. Nature. 2013, 495, 80-84.

Enhancement of CO_2 selectivity in a pillared pcu MOM platform through pillar substitution. Nugent, P.; Rhodus, V.; ***Pham, T.; Tudor, B.; Forrest, K.A.***; Wojtas, L.; Space, B.; Zaworotko, M.J. Chem. Commun., 2013, 49, 1606-1608.

Simulation of the Mechanism of Gas Sorption in a Metal–Organic Framework with Open Metal Sites: Molecular Hydrogen in PCN-61. ***Forrest, K.A.; Pham, T.; McLaughlin, K.; Belof, J.L.; Stern, A.C.***; Zaworotko, M.J.; Space, B. J. Phys. Chem. C, 2012, 116 (29), 15538–15549.

Highly Selective CO_2 Uptake in Uninodal 6-Connected “mmo” Nets Based upon MO_4^{2-} (M = Cr, Mo) Pillars. Mohamed, M.H.; Elsaidi, S.K.; Wojtas, L.; ***Pham, T.; Forrest, K.A.;*** *Tudor, B.*; Space, B.; Zaworotko, M.J. J. Am. Chem. Soc., 2012, 134 (48), 19556-19559.

Past Work as an Independent Investigator

A molecular H_2 potential for heterogeneous simulations including polarization and many-body van der Waals interactions. ***McLaughlin, K.; Cioce, C. R.; Belof, J. L.***; Space, B., J. Chem. Phys. 2012, 136 (19).

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A Distributed Hyperpolarizability Model for Liquid Water. ***Neipert, C.***; Space, B., Comput. Lett., 2007, 3 (111), 431-440.

Generalized Computational Time Correlation Function Approach: Quantifying Quadrupole Contributions to Vibrationally Resonant Second-Order Interface-Specific Optical Spectroscopies. ***Neipert, C.;*** Space, B.***; Roney, A. B.*** J. Phys. Chem. C, 2007, 117 (111), 8749–8756.

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A Novel Technique for the Measurement of Polarization-Specific Ultrafast Raman Responses Constantine, S.; Gardecki, J.A.; Zhou, Y.; Ziegler, ***Ji, X.***; Space, B. L.D. J. Phys. Chem. A, 2001, 105 (43), 9851–9898

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Other Topics

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Why We Bet in No-limit Hold 'em: a Failure of Intuition. Phillips, D. and Space, B. Two Plus Two Magazine Vol. 14, No. 5 2018, https://www.twoplustwo.com/magazine/issue161/

A ProAm Guide to Live Poker. Phillips, D.; Space, B. Two Plus Two Magazine Vol. 13, No. 4 2017, http://www.twoplustwo.com/magazine/issue148/

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Expectation and Thin Value in No-limit Hold 'em: Profit comes with Variance. Space, B. Two Plus Two Magazine Vol. 10, No. 9 2014, http://www.twoplustwo.com/magazine/issue117/

Making a life in the physical sciences. Space, B., Journal of Organizational Behavior 2008, 29 (6), 755-759.

Pedagogical Manuscripts

Alternative Derivation of the Partition Function for Generalized Ensembles.
Belof, J. L. and Space, B; Cornell University Library, arXiv preprint arXiv:1309.2017 2013

Educational Training

National Science Foundation, Computer and Information Science and Engineering CS&E 1993
Postodoctoral Fellow at Princeton University

Metacenter Computational Science Institute in Parallel Computing 1993
University of Illinois at Urbana-Champaign

NATO Advanced Study Institute 1992
Alghero, Italy

Charles Coulson Summer School in Theoretical Chemistry 1990
University of Oxford, Oxford, England

Memberships and Affiliations

American Chemical Society

American Association for the Advancement of Science

Heterodox Academy

Community Service and Social Contributions

Volunteer tutor

Volunteer speaker for community and science organizations

Science fair judge

Mentor and "big brother" to Maddox Shaw

Fundraiser / founder for Montessori scholarship program to provide educational opportunity

Conferences Attended

I have regularly presented at conferences including: Gordon Research Conferences, Telluride Science Research Conferences (attendee and organizer), American Chemical Society (attendee and organizer, local and national), CELTIC 2014-2017, CECAM and several other ad hoc national and international meetings.

I have given dozens of departmental seminars including a 2018 tour of Chinese universities.

Service to the scientific community

I have served as a reviewer for journals on a consistent basis. I have reviewed for all the major physical chemistry and material science disciplinary journals and occasionally for broader scope publications. I have been an ad hoc grant reviewer for the military, NSF, DOE and NEUP on a regular basis. I have reviewed for several private foundations on an annual basis. I have served as an NSF and DOE panelist several times.

Service to the university

I have served on over a hundred masters and doctoral committees and continue to serve on several. I was a member of the University Research Council and chaired the University Research Computing Committee for several years. I have served on Tenure and Promotion committees at the college level several times. I have participating in two ad-hoc dean searches for the Graduate School and was co-chair in college of Natural and Environmental sciences search.

Service to the department

I have chaired and served on many search committees for faculty and instructors of all levels. I was graduate coordinator for six years after designing and implementing a modern graduate program that is in place today. I was associate chair under Dr. Randy Larsen in his first term as chair and initiated work on a strategic plan for the department. I have served as an informal faculty mentor and helped young faculty especially with developing NSF Career Awards, all of which were ultimately funded. I served on and chaired the departmental Faculty Advisory Council that advises the chair and leads T&P evaluations. I have been an active and energetic faculty citizen.

Awards and Honors

Alumni Teaching Award 2002
University of South Florida

NSF Career Development Award 1998

Bayer School of Natural and Environmental Sciences Award for Excellence in Scholarship 1998
Duquesne University

National Science Foundation Research Experience for Undergraduates Award 1987

Funded Grants

NSF PI, Modeling of Metal Organic Materials (MOMs): Force Field Innovations and Applications with Impact, $420,000 2016 – 2019

ACS American Chemical Society, Petroleum Research Fund:
New Directions, $110,000 2016 – 2018

NSF Major Research Instrumentation (MRI) Grant MRI: Acquisition of a Computer Cluster for Computational Materials Research and Education at the University of South Florida and Partnering Institutions in Tampa Bay, $197,469. 2016

NSF PI, Molecularly Detailed Theories of Interfaces: Spectroscopy, $390,500 2012 – 2015

KAUST co-PI, KAUST-USF Materials Network, $1,500,000 2010 – 2013

URAD Draper Laboratories, co-PI on Development of Novel Porphyrin Based Chemical/ Biological Threat Agent Sensors, $200,000. 2010 - 2012

NSF Major Research Instrumentation (MRI) Grant MRI: Acquisition of a Computational Cluster for Research and Training at the University of South Florida in Partnership with Eckerd College and the University of Tampa, $499,999. 2008

DOE Co-PI on DOE Grant, Smart Porous Metal-Organic Frameworks for Hydrogen Storage and Recovery, $882,000 2007 – 2011

NSF Co-PI on Stem Grant, Scholarships Reinforcing Computational Physical Science, $500,000 2006 – 2011

ACS American Chemical Society, Petroleum Research Fund, Type AC, $80,000 2005 – 2009

NASA Co-PI, Smart Porous Metal-Organic Frameworks for Hydrogen Recovery & Storage, $300,000 2005 – 2007

NSF PI, Theoretical Investigations of the Spectroscopy and the Associated Structure and Dynamics of Liquids and Their Interfaces, $345,000 2003 – 2007

NSF REU, Co-PI, Integrated Interdisciplinary Nanoscience REU, $213,000 2003 – 2006

ACS American Chemical Society, Petroleum Research Fund, Type AC, $80,000 2003 – 2005

ACS American Chemical Society, Petroleum Research Fund, Type AC, $60,000 2001 – 2003

NSF Chemistry Research Instrumentation and Facilities Grant Acquisition of Computer Equipment for an Advanced Parallel Computing Facility, $110,000 1999

NSF Career Development Award, Theoretical Studies of Condensed Phase Conduction and Spectroscopic Processes, $294,560 1998 – 2002

ACS American Chemical Society, Petroleum Research Fund, Type G, $20,000 1996 – 1997

Duquesne University Faculty Development Award for $4,615 1996

NIST Subcontractor on successful NIST grant with Moldyn Inc. to develop accelerated molecular dynamics techniques for polymers and proteins, $27,000 1995 – 1997

NSF Computational Science and Engineering Postdoctoral Research Associateship, 2 years of support totaling $45,056 1993 – 1995

NSF National Science Foundation International Travel Award, $1,000 1992

References

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Professor Klein is a FRS & National Academy member and chemical physics theory and simulation founder.

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Professor Straub is a leading biophysical theorist who is familiar with my career and accomplishments.

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Dr. Belof is a former doctoral student and ongoing collaborator that can provide a perspective of my abilities from a variety of perspectives. He has reached a high level as an independent scientist and is a productive classified and public domain material scientist with a large research group.

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Professor Thomas Isenhour is my first chair. He has a long history in academia having help several chair positions including at U.N.C. Chapel Hill. He has been Dean and Provost at multiple major universities. He is familiar with both my career and leadership abilities. He was most recently at Old Dominion University where he was Provost and a member of the chemistry department.

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Professor Larsen is an accomplished biophyscist, longtime colleague, collaborator and administrator.

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Professor Keyes is a leading theoretician that has both competed and collaborated with me in the past.