

# CURRICULUM VITAE

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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 conceiving 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** 2006 – 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<sub>2</sub> 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  $\pi$ -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<sub>2</sub> 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 Ita 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<sub>2</sub>H<sub>2</sub> Sorption in a-[M<sub>3</sub>(O<sub>2</sub>CH)<sub>6</sub>] (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.aag1636.
- Theoretical study of the effect of halogen substitution in molecular porous materials for CO<sub>2</sub> and C<sub>2</sub>H<sub>2</sub> sorption. **Franz, D. M.**; *Djulfbegovic, M.*; **Pham, T.**; Space, B. *AIMS Mater. Sci.* 2018, 5 (2), 226–245.
- Impact of partial interpenetration in a hybrid ultramicroporous material on C<sub>2</sub>H<sub>2</sub>/C<sub>2</sub>H<sub>4</sub> 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<sub>2</sub> 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<sub>2</sub>H<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub>H<sub>2</sub> from CO<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub>H<sub>2</sub>/CO<sub>2</sub> and CO<sub>2</sub>/C<sub>2</sub>H<sub>2</sub> 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<sub>2</sub> and H<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub>. 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<sub>2</sub> 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<sub>2</sub> 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.**; Schaefer, 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<sub>2</sub> sorption characteristics in a Mg<sup>2+</sup>-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<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> 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-bis(4-pyridyl)acetylene)<sub>2</sub>(Cr<sub>2</sub>O<sub>7</sub>)]<sub>n</sub>. 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<sub>2</sub> 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<sub>2</sub> 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  $\pi$ -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<sub>2</sub> 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<sub>2</sub> Sorption Mechanisms. **Pham, T.**; **Forrest, K. A.**; **McDonald, K.**; Space, B. Cryst. Growth Des. 2014, 14, 5599–5607.

- Capturing the H<sub>2</sub>–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  $\pi$ -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<sub>2</sub> and CH<sub>4</sub> Sorption in an Interpenetrated Diamondoid Metal–Organic Material. Pham, **T.; Forrest, K. A.; Tudor, B.**; Elsaïdi, 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<sub>4</sub> and CO<sub>2</sub> through Control over Interpenetration in Diamondoid Nets. Elsaïdi, 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.
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- A Polarizable and Transferable PHAST N<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> affinity in “mmo” topology networks. Mohamed, M.H.; Elsaïdi, 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<sub>2</sub> Sorption in [Cu(bpy)<sub>2</sub>SiF<sub>6</sub>]. **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<sub>2</sub> 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.
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*Past Work as an Independent Investigator*

- A molecular H<sub>2</sub> 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).
- Erratum: “A molecular H<sub>2</sub> potential for heterogeneous simulations including polarization and many-body van der Waals interactions” [*J. Chem. Phys.* 136, 194302 (2012)]. **McLaughlin, K.; Cioce, C. R.; Belof, J. L.**; Space, B., *J. Chem. Phys.* 2012, 137 (12), 129901.
- Understanding hydrogen sorption in a polar metal-organic framework with constricted channels **Stern, A. C.; Belof, J. L.**; Eddaoudi, M.; Space, B., *J. Chem. Phys.* 2012, 136, 034705.
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- Characterization of Tunable Radical Metal-Carbenes: Key Intermediates in Catalytic Cyclopropanation. **Belof, J. L.; Cioce, C. R.**; Xu, X.; Zhang, X. P.; Space, B.; Woodcock, H. L., *Organometallics* 2011, 30 (10), 2739-2746.

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- Evidence for Substrate Preorganization in the Peptidylglycine  $\alpha$ -Amidating Monooxygenase Reaction Describing the Contribution of Ground State Structure to Hydrogen Tunneling. McIntyre, N. R.; Lowe, E. W.; **Belof, J. L.**; Ivkovic, M.; Shafer, J.; Space, B.; Merkle, D. J., J. Am. Chem. Soc. 2010, 132 (46), 16393-16402.
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- A Predictive Model of Hydrogen Sorption for Metal-Organic Materials. **Belof, J. L.**; **Stern, A. C.**; Space, B., J. Phys. Chem. C 2009, 113 (21), 9316-9320.
- Making a life in the physical sciences Space, B., Journal of Organizational Behavior 2008, 29 (6), 755-759.
- Photophysical Studies of the Trans to Cis Isomerization of the Push-Pull Molecule: 1-(Pyridin-4-yl)-2-(N-methylpyrrol-2-yl)ethene (mepepy). Mokdad, A.; **Belof, J. L.**; Yi, S. W.; Shuler, S. E.; McLaughlin, M. L.; Space, B.; Larsen, R. W., J. Phys. Chem. A 2008, 112 (36), 8310-8315.
- An Accurate and Transferable Intermolecular Diatomic Hydrogen Potential for Condensed Phase Simulation. **Belof, J. L.**; **Stern, A. C.**; Space, B., J. Chem. Theory Comput. 2008, 4 (8), 1332-1337.
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- 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.
- A combined photothermal and molecular dynamics method for determining molecular volume changes. **Ridley, C.**; **Stern, A. C.**; **Green, T.**; **DeVane, R.**; Space, B.; Miksovskaya, J.; Larsen, R. W., Chemical Physics Letters 2006, 418 (1-3), 137-141.
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Over Betting Polarized Ranges in the Short Run: How Big to Bet? Space, B. Two Plus Two Magazine Vol. 12, No. 2 2016, <http://www.twoplustwo.com/magazine/issue134/>

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 Postdoctoral Fellow at Princeton University 1993

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

NATO Advanced Study Institute Alghero, Italy 1992

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

### **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 University of South Florida	2002
NSF Career Development Award	1998
Bayer School of Natural and Environmental Sciences Award for Excellence in Scholarship Duquesne University	1998
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**

### **Mike Zaworotko**

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*Dr. Zaworotko is a leading materials experimentalist and collaborator.*

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

**Dr. John E. Straub**

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

**Jon Belof, Ph.D.**

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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.*

**Thomas Isenhour, Ph.D.**

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*Professor Thomas Isenhour is my first chair. He has a long history in academia having held 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.*

**Randy William Larsen, PhD**

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

**Professor Tom Keyes**

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