

Brian Space, Ph.D.

Work Address

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PRESENT POSITION

University of South Florida, Department of Chemistry

Professor of Chemistry

Previous Experience

2000-2006 University of South Florida, Department of Chemistry

Associate Professor of Chemistry

1995-2000 Duquesne University, Department of Chemistry

Assistant Professor of Chemistry

1992-1995 Princeton University, Department of Chemistry

National Science Foundation, Computational Science and Engineering (CS&E) Postdoctoral Research
Associate with Professor Herschel Rabitz

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

1988-1992 Ph.D. in Chemistry, Boston University, with Professor David Coker

- Dissertation titled “Energetics and Dynamics of Excess Electrons in Simple Fluids”

1984-1988 B.A. in Chemistry, Boston University

- Performed experimental and theoretical research with Professor Erwin Poliakoff on photoionization of small molecules

Five Products Most Closely Related to Proposal

Space Group Graduate Student authors are shown in green.

Porous materials with optimal adsorption thermodynamics and kinetics for CO₂ separations by P. Nugent, Y. Belmabkhout, S.D. Burd, A.J. Cairns, R. Luebke, [K.A. Forrest](#), [T. Pham](#), S. Ma, Brian Space, L. Wojtas, M. Eddaoudi and M.; Zaworotko, *Nature* DOI: 10.1038/nature11893 (2013)

Enhancement of CO₂ selectivity in a pillared pcu MOM platform through pillar substitution by P. Nugent, V. Rhodus, [T. Pham](#), [B. Tudor](#), [K.A. Forrest](#), K.A., L. Wojtas, Brian Space and M.J. Zaworotko, *Chem. Comm.* **49** 1606 (2013)

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

Hydrogen adsorbed in a metal organic framework-5: Coupled translation-rotation eigenstates from quantum five-dimensional calculations by I. Matanovic, [Jonathan L. Belof](#), Brian Space, K. Sillar, J. Sauer, J. Eckert and Z. Bacic, *J. Chem. Phys.* **137** 014701 (2012)

A molecular H₂ potential for heterogeneous simulations including polarization and many-body van der Waals interactions by [K. McLaughlin](#), [C.R. Cioce](#), [J.L. Belof](#) and Brian Space, J. Chem. Phys. **136** 194302 (2012)

Five Other Significant Products

Understanding Hydrogen Sorption in a Polar Metal-Organic Material with constricted channels by [Jonathan L. Belof](#), [Abraham C. Stern](#), Mohamed Eddaoudi and Brian Space, J. Chem. Phys. **135** (2011)

Atomic Charges Derived from Electrostatic Potentials for Molecular and Periodic Systems by De-Li Chen, [Abe Stern](#), Brian Space and J. Karl Johnson, J. Phys. Chem. A **114** 10225-10233 (2009)

A Predictive Model of Gas Sorption for Metal-Organic Materials by [Jon Belof](#), [Abe Stern](#) and Brian Space, J. Phys. Chem. C **113** 9316-9320 (2009)

An Accurate and Transferable Intermolecular Diatomic Hydrogen Potential for Condensed Phase Simulation by [Jon Belof](#), [Abe Stern](#) and Brian Space, J. Chem. Theory and Comput **4** 1332-1337 (2009)

On the Mechanism of Hydrogen Storage in a Metal-Organic Framework (MOF) Material by [Abraham C. Stern](#), [Jonathan L. Belof](#), Mohamed Eddaoudi and Brian Space, J. Am. Chem. Soc **129** 15202-15210 (2007)

Synergistic Activities:

Member IDRIB Materials research cluster (<http://chemistry.usf.edu/department/tour/idrb/>) that is a locally housed group of 14 researchers from STEM fields participating in funded materials research; it consists of half theoretical and experimental researchers to promote effective collaboration.

Member of the state materials center USF SMMARTT (<http://chemistry.usf.edu/smmartt/>) with its stated mission: "To discover and develop new 'smart' metal-organic material (MOM) platforms for energy sustainability and enhancement of human health".

Recent Collaborators and Former Mentors:

David Coker - Boston University, Ph.D. adviser; Thomas la Cour Jansen - Rijksuniversiteit Groningen; Preston Moore - University of the Sciences in Philadelphia; Herschel Rabitz - Princeton University, postdoctoral adviser

Former Advisees:

Undergraduate Students:

[Giovanni Quiel](#)[†], Christian Cioce, Emilio Esposito, [Samantha Halpin](#)* (REU), [Abe Stern](#)[†], [Jarmymar Vazquez](#)[†] (REU)

Graduate Students:

[Dr. Heather Ahlborn](#), Dr. Russell DeVane, Dr. Jonathan Belof, Dr. Xingdong Ji, [Dr. Christina Ridley Kasprzyz](#), [Ms. Christine Neipert](#)[†], [Dr. Angela Perry](#), Dr. Ben Roney, [Dr. Abe Stern](#),[†] Dr. Jonathan L. Belof

Postdoctoral Associates: Dr. H.F. Bowen, [Dr. Vaishali Shah](#)

Current Advisees:

Graduate Students (5):

Christian Cioce, [Ms. Katherine A. Forrest](#), Mr. Keith McLoughlin, [Ms. Ashley Mullen](#), Mr. Tony Pham

Undergraduate Students (2):

[Mr. Kyle McDonald](#)[†], Mr. Brant Tudor

* Students in [blue](#) are members of underrepresented groups, [†] represents Hispanic students.