

Brian Space, Ph.D.

Work Address

University of South Florida
Department of Chemistry
4202 E. Fowler Ave., CHE 205
Tampa, FL 33620-5250
(813) 765-4846
E-mail: space@cas.usf.edu
<http://www.cas.usf.edu/chemistry/faculty/space.html>

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 Publications Most Closely Related to Proposal

Space Group Graduate Student authors are shown in green.

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)

A Time Correlation Function Theory Describing Static Field Enhanced Third Order Optical Effects at Interfaces by **Christine Neipert** and Brian Space, *J. Chem. Phys.* **125** 224706-11 (2007)

Five Other Significant Publications

A Distributed Hyperpolarizability Model for Liquid Water by [Christine Neipert](#) and Brian Space, *Comp. Lett.* **3** 431-440 (2007)

Generalized Computational Time Correlation Function Approach: Quantifying Quadrupole Contributions to Vibrationally Resonant Second-Order Interface-Specific Optical Spectroscopies by [Christine Neipert](#) and Brian Space, *J. Phys. Chem. C.* **111** 8749-56 (2007)

Evidence for Substrate Preorganization in the Peptidylglycine -Amidating Monooxygenase Reaction Describing the Contribution of Ground State Structure to Hydrogen Tunneling by Neil R. McIntyre, Edward W. Lowe, Jr., [Jonathan L. Belof](#), Milena Ivkovic, Jacob Shafer, Brian Space, and David J. Merkler *J. Am. Chem. Soc.* **132** 16292-16402 (2010)

Time correlation theories of nonlinear spectroscopy by Brian Space, *Lecture Series on Computer and Computational Science.* Brill Academic Publishers **7** 1231-1233 (2007)

Volume title: *Structure and Chemistry at Aqueous Interfaces*, Article title: *Theoretical Modeling of Interfacial Vibrational Spectroscopy: Methods and Applications to Aqueous Interfaces* by [Angela Perry](#), [Christine Neipert](#), Preston Moore and Brian Space, *Chemical Reviews* **106** 1234-1258 (2006)

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:

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†](#)

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. Giovanni Quiel†](#), Mr. Brant Tudor

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

Synergistic Activities:

co-PI with Professor David Rabson (USF Physics) on a \$500,000 **NSF S-STEM grant** “*SCHOLARSHIPS IN SCI, TECH, ENG, AND MATH: Scholarships Reinforcing Computational Physical Science.*” The programs aim is to increase the number of undergraduate students in computational science by supporting 25 students for four years of study. The program includes common core courses, the involvement of the scholars in high-performance computation research groups, and a recruitment program to involve African-American and Hispanic students, constituting 50% of USF’s catchment population, in STEM majors (currently being submitted for renewal).