

## CURRICULUM VITAE

**Kevin E. Riley**

Department of Chemistry

University of Puerto Rico, Rio Piedras Campus

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### EDUCATION

B.A. Chemistry, B.A. Physics, May 1999, University of New Mexico.

Ph.D. Theoretical Chemistry, December 2003, The Pennsylvania State University.

### EXPERIENCE

➤ August 2008 to present – Assistant Professor of Chemistry, University of Puerto Rico, Rio Piedras Campus.

- Studies of interactions between estrogen receptors ( $\alpha$  &  $\beta$ ), their ligands, and coactivators using classical molecular dynamics and dispersion augmented semiempirical techniques.
- High level computational studies on halogen bonding and  $\sigma$ -hole bonding complexes of relevance in biology.
- *Ab initio* and DFT-D studies of inter and intra-molecular interactions relevant to the structure, stability, and dynamics of proteins, protein-ligand complexes, and nucleic acids.
- High level computational studies on DNA/RNA interactions and the binding of variously substituted intercalators.

➤ July 2007 to July 2008 – Junior Research Associate, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic.

- *Ab initio* and DFT-D studies of inter and intra-molecular interactions relevant to the structure and stability of proteins and protein-ligand complexes
- MP2, coupled cluster, and density functional symmetry adapted perturbation theory studies of halogen bonding in biological systems
- Molecular dynamics and DFT-D studies of the interactions between the TATA box binding protein and DNA

➤ January 2007 through June 2007 – Post doctoral research fellow with Professor Pavel Hobza, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic.

- *Ab initio* and DFT-D studies of inter and intra-molecular interactions relevant to the structure and stability of proteins and protein-ligand complexes
- Coupled cluster and symmetry adapted perturbation theory studies of halogen bonding in small model complexes
- Development of DFT-D technique that takes into account environmental effects (ie solvation)
- DFT-D studies of the activated and inactivated mineralocorticoid nuclear receptor complexed with several agonists and antagonists

➤ January 2004 through December 2006 – Post doctoral research assistant with Professor Kenneth M. Merz:

- January 2004 through June 2005 – Department of Chemistry, The Pennsylvania State University
- July 2005 through December 2006 – Department of Chemistry and Quantum Theory Project, The University of Florida

- Development of new functionals for use in Density Functional Theory
- High quality, *ab initio*, potential energy curves for interactions between weakly bound systems
- *Ab initio* and semiempirical studies of inter and intra-molecular interactions relevant to the structure and stability of proteins and protein-ligand complexes

➤ September 1999 through December 2003 – Graduate research assistant with Professor James B. Anderson, Department of Chemistry, The Pennsylvania State University.

- Quantum Monte Carlo Potential energy surfaces for reactions of small molecules
- Development of new sampling functions for use with Quantum Monte Carlo
- Variational Monte Carlo gradient techniques for geometry optimization and other differential properties
- Development of new methods to determine configuration interaction coefficients using Variational Monte Carlo

➤ May 2000 through September 2000 – Visiting graduate student with Dr. Arne Lüchow, Institut für Physikalische Chemie und Elektrochemie, Heinrich Heine Universität, Düsseldorf.

- Development of new methods to determine configuration interaction coefficients using Variational Monte Carlo

➤ September 1999 to December 1999 – Teaching assistant for General Chemistry laboratory, The Pennsylvania State University.

➤ September 1996 through May 1999 – Undergraduate research assistant with Professor David Keller, Department of Chemistry, University of New Mexico.

- Experimental studies on the interactions between actin and myosin proteins using atomic force microscopy
- Modeling of atomic force microscope cantilever vibrations using large scale models in viscous fluids

### **TEACHING EXPERIENCE**

- Fall 1999 – General Chemistry laboratory
- Spring 2009 – Physical Chemistry II lecture - Quantum mechanics, statistical mechanics, reaction kinetics
- Fall 2009 – Physical Chemistry I lecture - Thermodynamics

## RESEARCH INTERESTS

- Study of relationship between primary and secondary structure in proteins using semiempirical and *ab initio* electronic structure techniques.
- Study of weak intermolecular interactions by high quality *ab initio* methods.
- Study of protein-ligand interactions using molecular dynamic, semiempirical, and *ab initio* methods.
- Development of new DFT functionals and empirically derived DFT dispersion functions (DFT-D) well suited for electronic calculations of very large biological systems (ie: proteins and DNA).

## HONORS / AWARDS / SUPPORT

- ❖ 2009 – UPR-RP Institutional Research Fund Award (\$37,500), UPR-RP
- ❖ 2009 – Collaborator on NSF Partnership for Research and Education in Materials (PREM) Grant (Grant # 0934115, \$3,500,000), UPR-RP
- ❖ 2008 – Teragrid grant for 20,000 hours of supercomputer time (Grant #MCB090013), UPR-RP
- ❖ 2008 – NSF Institute for Functional Nanomaterials Faculty Start-up Award (\$150,000), UPR-RP
- ❖ 2006 – International Postdoctoral Fellowship, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
- ❖ 2002-2003 – IGERT Graduate Research Fellowship, The Pennsylvania State University
- ❖ 2003 – Geiger Graduate Research Award, The Pennsylvania State University
- ❖ 2003 – Delalian graduate Research Award, The Pennsylvania State University
- ❖ 1998 – REU-NSF Undergraduate Research Fellowship, University of New Mexico

## ADDITIONAL EDUCATION AND EXPERIENCE

- June 2009 – Visiting Scholar, Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences.
- May 2009 to present – Reviewer for *Journal of Chemical Physics*.
- October 2008 to present – Undergraduate research advisor to Eduardo Vega, Ety Vazquez, Felix Ramos, and Jose-Carlos Iglesias, UPR-RP.
- January 2009 to present – Graduate research co-advisor to Yamixa Delgado, UPR-RP.
- January 2009 to present – Member of master's thesis committee of Maitreyi Agarwal, UPR-RP.
- August 2008 to present – Member, Academic Affairs Committee, Department of Chemistry, UPR-RP.
- August 2008 to present – Member, subcommittee (Academic Affairs) for the establishment of a "Mathematics for Chemistry Students" course, UPR-RP.
- Spring/Summer 2007 – Member of Ph.D. thesis committee of Michal Hanus, Charles University, Prague; defense in June of 2007.
- October 2007 through present – Reviewer for *Journal of Molecular Modeling*.
- April 2006 through present – Reviewer for *Journal of Chemical Theory and Computation*.
- October 2006 through present – Reviewer for *International Journal of Quantum Chemistry*.
- Summer 2004 – Schreyer Institute for Teaching Excellence Certificate, at The Pennsylvania State University.

## PRESENTATIONS

- “Studies on Geometries of Various Intermolecular Interaction Motifs using Several Wavefunction- and Density Functional- Based Theories  
Kevin E. Riley  
A **poster** presented at the “Current Trends in Computational Chemistry” conference, Jackson, MS (October 2009)
- “Investigations on the Origins and Nature of Halogen Bonds by *Ab Initio* Methods”  
Kevin E. Riley  
An **invited oral presentation** presented at the Central Regional Meeting of the American Chemical Society, Cleveland, OH (May 2009).
- “The Contributions of Aromatic Interactions to the Structure and Stability of Amyloid Fibrils”  
Kevin E. Riley  
A **poster** presented at the “2009 Sanibel Conference”, St. Simon Island, GA (March 2009).
- “The Importance of Weak Interactions in Protein and Nucleic Acid Structure”  
Kevin E. Riley  
An **oral presentation** presented in the Department of Chemistry, University of Puerto Rico (Rio Piedras), San Juan, PR (December 2008).
- “Computational Treatment of Pi-Bonding Systems: How Well can we Describe Geometries”  
Kevin E. Riley  
An **invited oral presentation** presented at the “Vienna-Prague Quantum Chemistry Seminar”, Vienna, Austria (May 2008).
- “A Computational Investigation into the Interactions between Nucleobases and Substituted Benzene Dimers”  
Kevin E. Riley and Pavel Hobza  
A **poster** presented at the “Isolated Biomolecules and Biomolecular Interactions Conference”, Valladolid, Spain (April 2008).
- “High Accuracy *Ab Initio* Calculations Used to Describe Nucleic Acid Systems”  
Kevin E. Riley  
An **invited oral presentation** presented in the Department of Chemistry, University of Puerto Rico (Rio Piedras), San Juan, PR (March 2008).
- “High Accuracy *Ab Initio* Calculations Used to Describe Nucleic Acid Systems”  
Kevin E. Riley  
An **invited oral presentation** presented in the Department of Chemistry, Wright State University, Dayton, OH (March 2008).
- “Unusually Strong Interactions between Proline and Aromatic Residues”  
Kevin E. Riley, Lada Biedermanová, Jiří Vondrášek, and Pavel Hobza  
A **poster and short oral presentation** presented at the “2008 Sanibel Conference”, St. Simon Island, GA (February 2008).
- “The Use of Correlated Methods in Studies of Nucleic Acid Systems”  
Kevin E. Riley  
An **invited oral presentation** presented at the “Computational Group Seminar”, Department of Physical and Theoretical Chemistry, Comenius University, Bratislava, Slovakia (February 2008).
- “Investigations into the Nature of Halogen Bonds and their Significance in Biological Systems”  
Kevin E. Riley  
An **invited oral presentation** presented at the “Modeling Interactions in Biomolecules III” conference, Prague, Czech Republic (August 2007).

“Development of the DFT-D Method to Include Implicit Solvation and Applications to Steroid-Mineralocorticoid Receptor Interactions”

Kevin E. Riley

An **invited oral presentation** presented at the “Computational Chemistry Division Seminar”, National Institute for Standards and Technology, Gaithersburg, MD (June 2007)

“Halogen Bonding in Biological Complexes”

Kevin E. Riley and Pavel Hobza

A **poster** presented at the “Biological Molecules in the Gas Phase” Gordon Research Conference, Bates College, Lewiston, ME (June 2007).

“Investigations on Halogen Bonding in Biological Systems”

Kevin E. Riley

An **oral presentation** presented at the “Division of Molecular Modeling Seminar”, Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague, Czech Republic (January 2007).

“Critical Assessment of the Performance of Density Functional Theory Methods for Several Atomic and Molecular Properties”

Kevin E. Riley

An **invited oral presentation** presented at the “Workshop on the Future of Biomolecular Simulations”, Oak Ridge National Laboratory, Oak Ridge, TN (December 2006).

“*Ab Initio* Investigations on the Geometric Dependence of Various Halogen Bonds”

Kevin E. Riley

An **oral presentation** presented at the “Quantum Theory Project Seminar”, Quantum Theory Project, University of Florida, Gainesville, FL (September 2006).

“How well do Density Functional Methods Describe Heats of Formation, Ionization Potentials, and Electron Affinities of small molecules”

Kevin E. Riley, Bryan T. Op't Holt, and Kenneth M. Merz Jr.

A **poster and short oral presentation** presented at the “2006 Sanibel Conference”, St. Simon Island, GA (February 2006).

“Performance of Density Functional Methods for Describing Hydrogen Bonding”

Kevin E. Riley and Kenneth M. Merz Jr.

A **poster** presented at the “72<sup>nd</sup> Annual Meeting of the Southeastern Section of the American Physical Society (SESAPS)”, Gainesville, FL (November 2005).

“Effects of Fluorine Substitution on the Interactions of Edge-to-Face and Sandwich Configurations of the Benzene Dimer”

Kevin E. Riley and Kenneth M. Merz Jr.

A **poster and short oral presentation** presented at the “2005 Sanibel Conference”, St. Simon Island, GA (March 2005).

“Configuration Interaction Coefficients Generated by Variational Monte Carlo”

Kevin E. Riley and James B. Anderson

A **poster** presented at the “XI<sup>th</sup> International Conference of Quantum Chemistry 2003”, University of Bonn, Germany (July 2003).

“Time-Dependent Hartree-Fock Theory for the Evaluation of Hyperpolarizabilities of Small Atoms and Molecules”

Kevin E. Riley

An **oral presentation** presented at the “Physical Chemistry Seminar”, The Pennsylvania State University, State College, Pennsylvania (February 2001).

## PUBLICATIONS

“Noncovalent Interactions in Biochemistry”

Kevin E. Riley and Pavel Hobza, submitted to *Wiley Interdisciplinary Reviews: Computational Molecular Science*.

“Stabilization and Structure Calculations Based on Wave Function and Density Functional Theories: Extended Molecular Clusters ( $N \geq 24$ )”

Kevin E. Riley, Michal Pitoňák, Petr Jurečka, and Pavel Hobza, submitted to *Chem. Rev.*

“On the Structure and Geometry of Biomolecular Binding Motifs (H-Bonding, Stacking, X-H... $\pi$ , Dispersion): WFT and DFT Calculations”

Kevin E. Riley, Michal Pitoňák, Jiří Černý, and Pavel Hobza, *J. Chem. Theory Comput.*, **6**, 66 (2010).

“*Ab Initio* Studies of the Characteristics of Hydrogen Bonds Involving Aromatically Bound Hydroxyl and Amino Groups and the Effects of Fluorine Substitution on these Interactions”

Kevin E. Riley, accepted in *Int. J. Quantum Chem.*

“Br...O Complexes as Probes of Factors Affecting Halogen Bonding: Interactions of Bromobenzenes and Bromopyrimidines with Acetone”

Kevin E. Riley, Jane S. Murray, Peter Politzer, Monica C. Concha, and Pavel Hobza, *J. Chem. Theory Comput.*, **5**, 155-163 (2009).

“Reference Quantum Chemical Calculations on RNA Base Pairs Directly Involving the 2'-OH Group of Ribose”

Jiri Šponer, Marie Zgaarbova, Petr Jurecka, Kevin E. Riley, Judit E. Sponer, and Pavel Hobza, *J. Chem. Theory Comput.*, **5**, 1166-1179 (2009).

“Representative Amino Acid Side Chain Interactions In Proteins. A Comparison of Highly Accurate Correlated *ab Initio* Quantum Chemical and Empirical Potential Procedures”

Karel Berka, Roman Laskowski, Kevin E. Riley, Pavel Hobza, and Jiří Vondrášek, *J. Chem. Theory Comput.*, **5**, 982 (2009).

“Accurate CCSD(T) and DFT-SAPT Stabilization Energies of the H-bonded and Stacked Structures of the Uracil Dimer”

Michal Pitoňák, Kevin E. Riley, and Pavel Hobza, *ChemPhysChem*, **9**, 1636 (2008).

“Another Role of Proline: Stabilization Interactions in Proteins Involving Proline and Residues of Aromatic Character”

Lada Biedermannová, Kevin E. Riley, Pavel Hobza, and Jiří Vondrášek, *Phys. Chem. Chem. Phys.*, **10**, 6350 (2008).

“Nature and Magnitude of Aromatic Stacking of Nucleic Acid Bases”

Jiri Šponer, Kevin E. Riley, and Pavel Hobza, an invited “perspective” article in the special “Stacking Interactions” issue of *Phys. Chem. Chem. Phys.* **10**, 2595 (2008).

**(Points of note: 1)** This article was selected to be republished in *Chemical Biology Research Articles*, a journal that collects the top articles throughout all Royal Society of Chemistry publications. **2)** This article was one of a total of ten articles selected to be republished in the *Phys. Chem. Chem. Phys.* tenth anniversary issue.)

“A DFT-D Investigation of the Mechanisms for Activation of the Wild-Type and S810L Mutated Mineralocorticoid Receptor by Steroid Hormones”

Kevin E. Riley and Pavel Hobza, *J. Phys. Chem. B*, **112**, 3157 (2008).

“Investigations into the Nature of the Halogen Bond including Symmetry Adapted Perturbation Theory Analyses”

Kevin E. Riley and Pavel Hobza, *J. Chem. Theory Comput.*, **4**, 232 (2008).

“Performance of the DFT-D Method, Paired with the PCM Implicit Solvation Model, for the Computation of Interaction Energies of Solvated Complexes of Biological Interest”

Kevin E. Riley, Jiří Vondrášek, and Pavel Hobza, *Phys. Chem. Chem. Phys.*, **9**, 5555 (2007).

“Investigation into the Performance of the MP2 Method, along with Several Basis Sets, for the Computation of Interaction Energies of Biologically Relevant Nonbonding Complexes”

Kevin E. Riley and Pavel Hobza, *J. Phys. Chem. A*, **111**, 8257 (2007).

“Assessment of Density Functional Theory Methods for the Computation of Heats of Formation and Ionization Potentials of Systems Containing Third Row Transition Metals”

Kevin E. Riley and Kenneth M. Merz Jr., *J. Phys. Chem. A*, **111**, 6044 (2007).

“An *Ab Initio* Investigation of the Interactions Between the Set of Fluorinated N-(4-Sulfamylbenzoyl)benzylamine (SBB) Inhibitors and Human Carbonic Anhydrase II (HCAII)”

Kevin E. Riley, Guanglei Cui, and Kenneth M. Merz Jr., *J. Phys. Chem. B*, **111**, 5700 (2007).

“Insights into the Strength and Origin of Halogen Bonding: the Halobenzene-Formaldehyde Dimer”

Kevin E. Riley and Kenneth M. Merz Jr., *J. Phys. Chem. A*, **111**, 1688 (2007).

“Critical Assessment of the Performance of Density Functional Methods for Several Atomic and Molecular Properties”

Kevin E. Riley, Bryan T. Op't Holt, and Kenneth M. Merz Jr., *J. Chem. Theory Comput.* **3**, 407 (2007).

(**Point of note:** This was the fourth most widely accessed online article in this journal in 2007)

“The Role of Solvation in the Energy Stabilization Inside the Hydrophobic Core of the Protein Rubredoxin”

Kevin E. Riley and Kenneth M. Merz Jr., *J. Phys. Chem. B*, **110**, 15650 (2006).

“Effects of Fluorine Substitution on the Edge-to-Face Interactions of the Benzene Dimer”

Kevin E. Riley and Kenneth M. Merz Jr., *J. Phys. Chem. B*, **109**, 17752 (2005).

“Accurate Atomic and Molecular Calculations without Gradient Corrections: Scaled SVWNV Density Functional”

Kevin E. Riley, Edward N. Brothers, Kenneth B. Ayers, and Kenneth M. Merz Jr., *J. Chem. Theory Comput.*, **1**, 546 (2005).

“Pairwise Decomposition of Residue Interaction Energies Using Semiempirical Quantum Mechanical Methods in Studies of Protein-Ligand Interaction”

Kaushik Raha, Arjan van der Vaart, Kevin E. Riley, Martin B. Peters, Lance M. Westerhoff, Hwanho Kim, and Kenneth M. Merz Jr., *J. Am. Chem. Soc.*, **127**, 6583 (2005).

“A Self Consistent Method for the Generation of Configuration Interaction Coefficients Using Variational Monte Carlo”

Kevin E. Riley and James B. Anderson, *Mol. Phys.*, **101**, 3119 (2003).

“Higher Accuracy Quantum Monte Carlo Calculations of the Barrier for the H + H<sub>2</sub> Reaction”

Kevin E. Riley and James B. Anderson, *J. Chem. Phys.*, **118**, 2437 (2003).

“A new Variational Monte Carlo Trial Wavefunction with Directional Jastrow Functions”

Kevin E. Riley and James B. Anderson, *Chem. Phys. Lett.*, **366**, 153 (2002).