Curriculum Vitae

Dr. Robert Kalescky
Postdoctoral Research Fellow
E-mail: rkalescky@smu.edu
Phone (Office): 214-768-8635
Phone (Cell): 214-803-1552
Website: http://robert.kalescky.org
Address: Department of Chemistry
Southern Methodist University
P.O. Box 750314
3215 Daniel Avenue
Dallas, Texas 75275-0314

Expertise

- Programming in Fortran 77/95, C, C++, Objective-C, Python, Visual Basic
- Parallel programing using MPI, OpenMP, Pthreads, CUDA, OpenCL
- Scripting in Bash, CSH, AWK, Perl, sed, Tcl, Visual Basic for Applications
- Installation and application of quantum chemical and molecular dynamics programs on High Performance Computing (HPC) clusters and workstations:
  - Quantum chemical programs: Gaussian, Q-Chem, GAMESS, CFOUR, Molpro, NWChem, DIRAC, ORCA
  - Molecular dynamics programs: CHARMM, NAMD, LAMMPS, Amber, MPDyn, GROMACS, OpenMM
  - Molecular visualization programs: VMD, Chimera, Avogadro, IQmol, POV-Ray
  - Molecular desktop programs: Spartan, SYBYL
  - Calculation of: optimized geometries, transition states, reaction paths, potential energy surfaces, spectroscopic information, binding free energies
  - Quantum mechanical methods used: Hartree-Fock, Density Functional Theory, Möller-Plesset, Coupled Cluster
  - HPC clusters used: ManeFrame, SMUHPC, CATCO (SMU); Stampede (UT); Big Bird (UTD)
- 15 years administration experience in UNIX using Linux (Red Hat and Debian derivatives), Mac OS X, FreeBSD, and Solaris including installation and configuration
- 10 years high performance and scientific programming experience
- Structured writing and documentation in LaTeX, BibTeX, reStructuredText, Sphinx, MediaWiki, HTML
- Source code revision control using Git, Mercurial, Subversion

Programming Experience

- **covariance_plots**: Automated covariance analysis producing heat map and histogram plots based on an arbitrary selection of atoms using a language similar to that of CHARMM; Written in Python using NumPy, Matplotlib, and MDAnalysis modules
- **covar_path**: Automated parallel determination of allosteric pathways in proteins based on a covariance analysis using an arbitrary selection of atoms producing a pathway plot using Graphviz; Written in Python using NumPy, Matplotlib, NetworkX, and MDAnalysis modules
- **run**: Queue management specifically designed for the CATCO group's unique ScaleMP-based cluster using CPU and memory binding to improve job performance with automated calculation submission for commonly used quantum chemical programs; Written in C
- **conrun**: Similar automated job submission design as "run" for use with the Condor queue system used on SMUHPC; Written in Bash
- **local_mode_analysis**: Automated analysis of local mode calculations that produces normal mode decomposition bar diagrams, adiabatic connection scheme plots as either PDF or DataGraph files, normal mode decomposition and local mode analysis LaTeX tables; Written in Python with Objective-C bridge for producing DataGraph files and hosted in a Git repository; Object oriented design using NumPy and Matplotlib Python modules and custom designed quantum chemical output parsing and LaTeX formatting modules

- **cbs**: Automated calculation of 2- and 3-point complete basis set limits for arbitrary basis sets; Written in Python using NumPy module
- **molecular_connectivity**: Automated determination of all possible internal coordinate parameters and a unique non-redundant set of parameters based on symmetry for a given molecule; Written in Python using SciPy, NumPy, and NetworkX modules
- **Evolution**: Simple classical molecular dynamics program; Written in C++ using Pthreads for parallelization
- **SeisRoute**: Program for viewing and optimizing seismic vessel routes over oil fields based on weather and sea conditions; GUI program written in Visual Basic
- Numerous other tools to aid in analysis and running of quantum chemical programs: clean_directory, ganharmonic, gharmonic, gcartesian, gsymmetry, combine_irc, differentiate, gamess_gaussian_bridge, clean_cfour
- Development of automated coarse-grained molecular dynamics simulation system setup programs

Technical Workshop and Teaching Experience

- Advanced CHARMM Workshop, Spring 2014
- Advanced Python Programming Workshop, Fall 2014
- URVA Workshop 2014
- Graduate/Undergraduate Computational Chemistry Laboratory, Southern Methodist University, 2013
- LaTeX Workshop, Spring 2013
- Graduate/Undergraduate Computer Aided Drug Design Laboratory, Southern Methodist University, 2012
- CATCO Methods Workshop 2012
- CATCO URVA Workshop 2012
- Graduate/Undergraduate Computational Chemistry Laboratory, Southern Methodist University, 2011
- Graduate/Undergraduate Computer Aided Drug Design Laboratory, Southern Methodist University, 2010
- Undergraduate General Chemistry Laboratory, Southern Methodist University, 2010-2011
- Graduate/Undergraduate Computational Chemistry Laboratory, Southern Methodist University, 2009

Education

- Doctor of Philosophy in Chemistry, Southern Methodist University, 2009-2014, *Description of the Strength of Chemical Bonds Utilizing Local Vibrational Modes*
- Master of Science in Chemistry, University of Texas at Dallas, 2007-2009, *Area Per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach*
- Bachelor of Science in Chemical Engineering, Minors in Mathematics and Chemistry, Texas Tech University, 2001-2006, *Prairie Grass Ethanol Production Pilot Plant Facility and Optimization*

Research Experience

- Postdoctoral Research, Dr. Peng Tao, Southern Methodist University, 2014-Present
- Graduate Research, Dr. Elfi Kraka and Dr. Dieter Cremer, Southern Methodist University, 2009-2014
- Graduate Research, Dr. Steve Nielsen, University of Texas at Dallas, 2007-2008
- Undergraduate Research, Dr. Theodore Wiesner, Texas Tech University, 2006
- Undergraduate Research, Dr. Karlene Hoo, Texas Tech University, 2006
- Undergraduate Research, Dr. Jeremy Leggoe, Texas Tech University, 2005

Research Interests

- Parallelization development of HPC quantum chemical and classical molecular dynamics programs
- Development of high-throughput molecular dynamics analysis methods

- Characterization of chemical reaction involving proteins using chain-of-states and hybrid quantum and molecular mechanical methods
- Characterization of protein allostery using rigid body molecular dynamics
- Investigations of chemical bond strength using adiabatic force constants
- Investigations of chemical reactions using the united valley reaction approach
- Comparison of the chemical bond strength descriptors adiabatic force constants and compliance constants

Peer-Reviewed Publications

14. Kalescky, R.; Liu, J.; Tao, P. Identifying Key Residues for Protein Allostery through Rigid Residue Scan. *J. Phys. Chem. A* **2015**, *119*, 1689-1700.
13. Kalescky, R.; Zou, W.; Kraka, E.; Cremer, D. Quantitative Assessment of the Multiplicity of Carbon-Halogen Bonds: Carbenium and Halonium Ions with F, Cl, Br, and I. *J. Phys. Chem. A* **2014**, *118*, 1948–1963.
12. Kalescky, R.; Kraka, E.; Cremer, D. Accurate Determination of the Binding Energy of the Formic Acid Dimer: The Importance of Geometry Relaxation. *J. Chem. Phys.* **2014**, *140*, 084315.
11. Kalescky, R.; Kraka, E.; Cremer, D. Are Carbon-Halogen Double and Triple Bonds Possible? *Int. J. Quantum Chem.* **2014**, *114*, 1060–1072.
10. Kalescky, R.; Kraka, E.; Cremer, D. Description of Aromaticity with the Help of Vibrational Spectroscopy: Anthracene and Phenanthrene. *J. Phys. Chem. A* **2014**, *118*, 223–237.
9. Kalescky, R.; Kraka, E.; Cremer, D. New Approach to Tolman's Electronic Parameter Based on Local Vibrational Modes. *Inorg. Chem.* **2014**, *53*, 478–495.
8. Kalescky, R.; Zou, W.; Kraka, E.; Cremer, D. Vibrational Properties of the Isotopomers of the Water Dimer Derived From Experiment and Computations. *Aust. J. Chem.* **2014**, *67*, 426–434.
7. Kalescky, R.; Kraka, E.; Cremer, D. Identification of the Strongest Bonds in Chemistry. *J. Phys. Chem. A* **2013**, *117*, 8981–8995.
6. Kalescky, R.; Kraka, E.; Cremer, D. Local Vibrational Modes of the Formic Acid Dimer – The Strength of the Double Hydrogen Bond. *Mol. Phys.* **2013**, *111*, 1497–1510.
5. Zou, W.; Kalescky, R.; Kraka, E.; Cremer, D. Relating Normal Vibrational Modes to Local Vibrational Modes: Benzene and Naphthalene. *J. Mol. Model.* **2012**, *19*, 2865–2877.
4. Kalescky, R.; Zou, W.; Kraka, E.; Cremer, D. Local Vibrational Modes of the Water Dimer – Comparison of Theory and Experiment. *Chem. Phys. Lett.* **2012**, *554*, 243–247.
3. Zou, W.; Kalescky, R.; Kraka, E.; Cremer, D. Relating Normal Vibrational Modes to Local Vibrational Modes with the Help of an Adiabatic Connection Scheme. *J. Chem. Phys.* **2012**, *137*, 084114.
2. Ranatunga, U.; Kalescky, R.; Chiu, C.; Nielsen, S. Molecular Dynamics Simulations of Surfactant Functionalized Nanoparticles in the Vicinity of an Oil/Water Interface. *J. Phys. Chem. C* **2010**, *114*, 12151–12157.
1. Kalescky, R.; Shinoda, W.; Moore, P.; Nielsen, S. Area Per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach. *Langmuir* **2009**, *25*, 1352–1359.

Presentations

12. "Using Rigid Body Molecular Dynamics to Explore Key Residues of Protein Allostery", Southwest Regional Meeting of the American Chemical Society, Fort Worth, Texas, United States, November 22, 2014
11. "What are the Strongest Bonds in Chemistry", ASMD@D, Dallas, Texas, United States, March 4, 2014
10. "Description of the Strength of Chemical Bonds Utilizing Local Vibrational Modes" ", Chemistry Departmental Presentation, Southern Methodist University, January 24, 2014
9. "A Force Field for the Study of Small Molecule Absorption and Diffusion By Metal-Organic Frameworks in Fully Flexible Simulations", Chemistry Departmental Presentation, Southern Methodist University, January 22, 2013
8. "Description of the Strength of Carbon-Halogen and Carbon-Chalcogen Bonds Utilizing Local Vibrational Modes", Chirality 2012, Fort Worth, Texas, United States, June 11, 2012
7. "Exotic Carbon-Halogen Bonds Described By Local Vibrational Modes", ASMD@D, Dallas, Texas, United States, March 6, 2012

6. "Description of the Strength of Carbon-Halogen and Carbon-Chalcogen Bonds Utilizing Local Vibrational Modes", Chemistry Departmental Presentation, Southern Methodist University, October 26, 2011
5. "Carbon Nanotubes: Structure, Properties, and Controlled Synthesis", Chemistry Departmental Presentation, Southern Methodist University, November 12, 2010
4. "Area per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach", Chemistry Departmental Presentation, University of Texas at Dallas, April 21, 2009
3. "Correlating Surfactant Hydrophilic-Lipophilic Balance and Nanoparticle Radii via Coarse‐Grained Molecular Dynamics Simulations", 41st meeting of the Dallas-Fort Worth Local Section of the American Chemical Society, Dallas, United States, April 19, 2008
2. "Correlating Surfactant Hydrophilic-Lipophilic Balance and Nanoparticle Radii via Coarse‐Grained Molecular Dynamics Simulations", 235th meeting of the American Chemical Society, New Orleans, United States, April 9, 2008
1. "Area per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach", Chem-Bio Symposium, University of Texas at Dallas, March 26, 2008

Scientific and Academic Service

- Designed book cover image for *Fundamentals of Controlled/Living Radical Polymerization*; Tsarevsky, N. V.; Sumerlin, B. S., Eds.; The Royal Society of Chemistry, 2013; pp. P001–P364.
- Graduate Student Assembly Representative (Southern Methodist University, Department of Chemistry) – August 2011 to August 2013
- Introduction to Computational Chemistry for High School Instructors 2011
- Graduate Student Symposium Planning Committee Member (American Chemical Society) – Fall 2011
- Chemistry Graduate Council Treasurer (Southern Methodist University) – 2011
- American Chemical Society Graduate Student Symposium Planning Committee – Spring 2011
- Chemistry Graduate Council Secretary (Southern Methodist University) – 2010

Awards and Honors

- 1st Place Poster Competition for Chemistry, Research Day, Southern Methodist University, February 10, 2012
- 2nd Place Poster Competition, Chem-Bio Symposium, University of Texas at Dallas, March 26, 2008
- Four-year varsity letterman; co-captain of the Texas Tech cross country and track teams – August 2001 to May 2005
- Recognized by Texas Tech University and the Big 12 Conference for excellence as a student athlete

Professional Experience

- Peloton Asset and Loan Services: Corporate IT support; built and maintained website, email, file, VPN, and offsite-backup servers, November 2008 to August 2010
- Schlumberger: Statistical data quality control of seismic GPS data, Model development for optimizing seismic vessel routes, May 2006 to June 2007
- Texas Tech University IT Help Central: Campus IT helpdesk student managerial position responsible for overseeing/helping student analysts, June 2005 to April 2006