ROBERT J. B. KALESCKY

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EDUCATION

Doctor of Philosophy in Chemistry – Southern Methodist University – May 2014
- Computational Chemistry concentration

Master of Science in Chemistry – University of Texas at Dallas – May 2009
- Computational Chemistry concentration

Bachelor of Science in Chemical Engineering – Texas Tech University – May 2006
- Mathematics and Chemistry minors

PROFESSIONAL EXPERIENCE

Postdoctoral Research Fellow – Southern Methodist University – January 2014 to Present
- Development of rigid body molecular dynamics method to explore protein allostery
- Python, Fortran, and parallelization programming
- Conducted programming and high performance computing seminars

Graduate Research Assistant – Southern Methodist University – August 2009 to January 2014
- Development of automated analysis methodologies for the study of the strength of chemical bonds
- C, Fortran, Python, Objective-C, and Bash programming

Graduate Research Assistant – University of Texas at Dallas – August 2007 to May 2009
- Development of automated coarse-grained molecular dynamics simulation system setup programs
- C, C++, and Bash programming

Peloton Asset and Loan Services – November 2008 to August 2010
- Corporate IT support; built and maintained website, email, file, VPN, and offsite-backup servers

Schlumberger – May 2006 to June 2007
- Statistical data quality control of seismic GPS data
- Model development for optimizing seismic vessel routes

IT Help Central – Texas Tech University – June 2005 to April 2006
- Campus IT helpdesk student managerial position responsible for overseeing/helping student analysts

COMPUTER KNOWLEDGE AND EXPERIENCE

UNIX (Linux, Mac OS X, Solaris)	High Performance Computing	Parallelization (MPI, OpenMP)	Microsoft Windows (Server)
C, C++, Objective-C, Fortran, Python	Shell Scripting (Bash, CSH, AWK)	MATLAB, Maple, Mathematica	Microsoft Office and LaTeX

PEER-REVIEWED PUBLICATIONS

17. Kalescky, R.; Liu, J.; Tao, P. Identification of Allosteric Pathways in PDZ2 Via Rigid Residue Scan. *J. Chem. Theory Comput.* **2015**, In Preparation.
16. Kalescky, R.; Liu, J.; Tao, P. Identifying Key Residues for Protein Allostery through Rigid Residue Scan. *J. Phys. Chem. A* **2014**, Accepted.
15. Kalescky, R. Description of the Strength of Chemical Bonds Utilizing Local Vibrational Modes. Ph.D. Dissertation, Southern Methodist University, Dallas, TX, **2014**.
14. 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.
13. 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.
12. Kalescky, R.; Kraka, E.; Cremer, D. Are Carbon-Halogen Double and Triple Bonds Possible? *Int. J. Quantum Chem.* **2014**, *114*, 1060–1072.
11. 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.
10. Kalescky, R.; Kraka, E.; Cremer, D. New Approach to Tolman's Electronic Parameter Based on Local Vibrational Modes. *Inorg. Chem.* **2014**, *53*, 478–495.
9. 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.
8. Kalescky, R.; Kraka, E.; Cremer, D. Identification of the Strongest Bonds in Chemistry. *J. Phys. Chem. A* **2013**, *117*, 8981–8995.
7. 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.
6. 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.
5. 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.
4. 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.
3. 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.
2. Kalescky, R. Area Per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach. M.S. Thesis, University of Texas at Dallas, Dallas, TX, **2009**.
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.

ACHIEVEMENTS AND EXTRACURRICULAR ACTIVITIES

- Graduate Student Assembly Representative (Southern Methodist University, Department of Chemistry) – August 2011 to August 2013
- Graduate Student Symposium Planning Committee Member (American Chemical Society) – Fall 2011
- Chemistry Graduate Council Treasurer (Southern Methodist University) – 2011
- Chemistry Graduate Council Secretary (Southern Methodist University) – 2010
- 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