Dr. Robert J. B. Kalescky

Curriculum Vitae, October 2018

HPC Applications Scientist
Center for Scientific Computation
Southern Methodist University
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Dallas, Texas 75205

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Research Interests

- Machine Learning Model Development for *ab initio* Molecular Dynamics
- Computational Material Design for Small Molecule Sieving Applications
- Computational Material Design for Nano-Scale Flow Reactors

Education

Doctor of Philosophy in Chemistry
Southern Methodist University, Dallas, Texas
August 2009 to May 2014
Description of the Strength of Chemical Bonds Utilizing Local Vibrational Modes

Master of Science in Chemistry
University of Texas at Dallas, Dallas, Texas
August 2007 to May 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, Lubbock, Texas
August 2001 to May 2006
Prairie Grass Ethanol Production Pilot Plant Facility and Optimization

Research Experience

HPC Applications Scientist — May 2015 to Present
Center for Scientific Computation
Southern Methodist University, Dallas, Texas

Postdoctoral Fellow — January 2014 to May 2015
Advising Professor: Dr. Peng Tao
Southern Methodist University, Dallas, Texas

Doctor of Philosophy in Chemistry Candidate — August 2009 to December 2014
Advising Professors: Dr. Elfi Kraka and Dr. Dieter Cremer
Computational and Theoretical Chemistry Group (CATCO)
Southern Methodist University, Dallas, Texas

Master of Science in Chemistry Candidate — August 2007 to May 2009
Advising Professor: Dr. Steven Nielsen
University of Texas at Dallas, Dallas, Texas

Publications

(17) Kalescky, R.; Zhou, H.; Liu, J.; Tao, P. Rigid Residue Scan Simulations Systematically Reveal Residue Entropic Roles in Protein Allostery. *PLoS Comput Biol* **2016**, *12*, 1–21.

(16) Neeman, H.; Bergstrom, A.; Brunson, D.; Ganote, C.; Gray, Z.; Guilfoos, B.; Kalescky, R.; Lemley, E.; Moore, B. G.; Ramadugu, S. K.; Romanella, A.; Rush, J.; Sherman, A. H.; Stengel, B.; Voss, D. In *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*, ACM: Miami, USA, 2016, 57:1–57:8.

(15) Setiawan, D.; Kalescky, R.; Kraka, E.; Cremer, D. Direct Measure of Metal–Ligand Bonding Replacing the Tolman Electronic Parameter. *Inorganic Chemistry* **2016**, *55*, 2332–2344.

(14) Kalescky, R.; Liu, J.; Tao, P. Identifying Key Residues for Protein Allostery through Rigid Residue Scan. *The Journal of Physical Chemistry A* **2015**, *119*, 1689–1700.

(13) Kalescky, R.; Kraka, E.; Cremer, D. Accurate determination of the binding energy of the formic acid dimer: The importance of geometry relaxation. *The Journal of Chemical Physics* **2014**, *140*, DOI: http://dx.doi.org/10.1063/1.4866696.

(12) Kalescky, R.; Kraka, E.; Cremer, D. Are carbon—halogen double and triple bonds possible? *International Journal of Quantum Chemistry* **2014**, *114*, 1060–1072.

(11) Kalescky, R.; Kraka, E.; Cremer, D. Description of Aromaticity with the Help of Vibrational Spectroscopy: Anthracene and Phenanthrene. *The Journal of Physical Chemistry A* **2014**, *118*, 223–237.

(10) Kalescky, R.; Kraka, E.; Cremer, D. New Approach to Tolman's Electronic Parameter Based on Local Vibrational Modes. *Inorganic Chemistry* **2014**, *53*, 478–495.

(9) 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. *The Journal of Physical Chemistry A* **2014**, *118*, 1948–1963.

(8) Kalescky, R.; Zou, W.; Kraka, E.; Cremer, D. Vibrational Properties of the Isotopomers of the Water Dimer Derived from Experiment and Computations. *Australian Journal of Chemistry* **2014**, *67*, 426–434.

(7) Kalescky, R.; Kraka, E.; Cremer, D. Local vibrational modes of the formic acid dimer – the strength of the double hydrogen bond. *Molecular Physics* **2013**, *111*, 1497–1510.

(6) Kalescky, R.; Kraka, E.; Cremer, D. Identification of the Strongest Bonds in Chemistry. *The Journal of Physical Chemistry A* **2013**, *117*, 8981–8995.

(5) Zou, W.; Kalescky, R.; Kraka, E.; Cremer, D. Relating normal vibrational modes to local vibrational modes: benzene and naphthalene. *Journal of Molecular Modeling* **2013**, *19*, 2865–2877.

(4) Kalescky, R.; Zou, W.; Kraka, E.; Cremer, D. Local vibrational modes of the water dimer – Comparison of theory and experiment. *Chemical Physics Letters* **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. *The Journal of Chemical Physics* **2012**, *137*, DOI: http://dx.doi.org/10.1063/1.4747339.

(2) Udayana Ranatunga, R. J. K.; Kalescky, R. J. B.; Chiu, C.-c.; Nielsen, S. O. Molecular Dynamics Simulations of Surfactant Functionalized Nanoparticles in the Vicinity of an Oil/Water Interface. *The Journal of Physical Chemistry C* **2010**, *114*, 12151–12157.

(1) Kalescky, R. J. B.; Shinoda, W.; Moore, P. B.; Nielsen, S. O. Area per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach. *Langmuir* **2009**, *25*, 1352–1359.

Conference Presentations

(14) Evaluation of DFT Dispersion Corrections on Hydrogen Isotopologue Separation in Metal-Organic Frameworks., Presentation, Austin Symposium of Molecular Structure and Dynamics, 2018.

(13) Hydrogen Isotopologue Separation in CPO-27-X., Poster, Austin Symposium of Molecular Structure and Dynamics, 2018.

(12) Description of the Strength of Chemical Bonds Utilizing Local Vibrational Modes., Presentation, Southern Methodist University, Department of Chemistry, 2014.

(11) Using Rigid Body Molecular Dynamics to Explore Key Residues of Protein Allostery., Presentation, Southwest Regional Meeting of the American Chemical Society, 2014.

(10) What are the Strongest Bonds in Chemistry., Poster, Austin Symposium of Molecular Structure and Dynamics, 2014.

(9) A Force Field for the Study of Small Molecule Absorption and Diffusion By Metal-Organic Frameworks in Fully Flexible Simulations., Presentation, Southern Methodist University, Department of Chemistry, 2013.

(8) Description of the Strength of Carbon-Halogen and Carbon-Chalcogen Bonds Utilizing Local Vibrational Modes., Presentation, Chirality, 2012.

(7) Exotic Carbon-Halogen Bonds Described By Local Vibrational Modes., Poster, Austin Symposium of Molecular Structure and Dynamics, 2012.

(6) Description of the Strength of Carbon-Halogen and Carbon-Chalcogen Bonds Utilizing Local Vibrational Modes., Presentation, Southern Methodist University, Department of Chemistry, 2011.

(5) Carbon Nanotubes: Structure, Properties, and Controlled Synthesis., Presentation, Southern Methodist University, Department of Chemistry, 2010.

(4) Area per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach., Presentation, University of Texas at Dallas, Department of Chemistry, 2009.

(3) Area per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach., Poster, Chem-Bio Symposium, 2008.

(2) Correlating Surfactant Hydrophilic-Lipophilic Balance and Nanoparticle Radii via Coarse-Grained Molecular Dynamics Simulations., Presentation, Dallas/Fort Worth Local American Chemical Society Meeting, 2008.

(1) Correlating Surfactant Hydrophilic-Lipophilic Balance and Nanoparticle Radii via Coarse-Grained Molecular Dynamics Simulations., Presentation, American Chemical Society, 2008.

Conferences and Workshops Attended

(16) Austin Symposium of Molecular Structure and Dynamics., Dallas, Texas, U.S. 2018.

(15) Super Computing 2017., Denver, Colorado, U.S. 2017.

(14) Advanced Cyber Infrastructure – Research and Educatation Facilitators., University of Oklahoma, Norman, Oklahoma, U.S. 2016.

(13) International Conference on Computational Science (ICCS)., University of California at San Diego and San Diego Supercomputer Center (SDSC), San Diego, California, U.S. 2016.

(12) S2SI High-Energy Physics and Computer Science., University of Illinois at Urbana–Champaign, Urbana and Champaign, Illinois, U.S. 2016.

(11) Super Computing 2016., Salt Lake City, Utah, U.S. 2016.

(10) Advanced Cyber Infrastructure – Research and Educatation Facilitators., University of Oklahoma, Norman, Oklahoma, U.S. 2015.

(9) Super Computing 2015., Austin, Texas, U.S. 2015.

(8) Austin Symposium of Molecular Structure and Dynamics., Dallas, Texas, U.S. 2014.

(7) Southwest Regional Meeting of the American Chemical Society., Fort Worth, Texas, U.S. 2014.

(6) Austin Symposium of Molecular Structure and Dynamics., Dallas, Texas, U.S. 2012.

(5) Chirality 2012., Fort Worth, Texas, U.S. 2012.

(4) 242nd American Chemical Society National Meeting., Denver, Colorado, U.S. 2011.

(3) 235th American Chemical Society National Meeting., New Orleans, Louisiana, U.S. 2008.

(2) Chem-Bio Symposium., University of Texas at Dallas, Dallas, Texas, U.S. 2008.

(1) Dallas/Fort Worth Local American Chemical Society Meeting., Southern Methodist University, Dallas, Texas, U.S. 2008.

Invited Seminar Presentations

(6) Using Jupyter Lab on M2., Presentation, Southern Methodist University, Department of Computer Science and Engineering, 2018.

(5) Accelerated Computations on ManeFrame II., Presentation, Southern Methodist University, Department of Computer Science and Engineering, Graduate Seminar, 2017.

(4) Supercomputing at SMU: An Introduction to ManeFrame., Presentation, Southern Methodist University, Department of Statistical Science, Graduate Seminar, 2017.

(3) Introduction to High Performance Computing, ManeFrame, and Applications., Presentation, Southern Methodist University, Department of Computer Science and Engineering, Graduate Seminar, 2016.

(2) ManeFrame Introduction., Presentation, Southern Methodist University, Department of Physics, Graduate Seminar, 2016.

(1) ManeFrame Introduction for Economics., Presentation, Southern Methodist University, Department of Economics, Graduate Seminar, 2016.

Technical Workshops and Teaching

2018

- Center for Scientific Computation Fall Workshop Series — 14 2-hour workshops
  1. ManeFrame II (M2) Introduction 2. Open Help Session 3. ManeFrame II (M2) Introduction 4. Parallel R on M2 5. Using Spack for Development 6. Open Help Session 7. ManeFrame II (M2) Introduction 8. OpenMP Introduction 9. OpenACC Introduction 10. MPI Introduction 11. Open Help Session 12. ManeFrame II (M2) Introduction 13. Parallel Python on M2 14. Open Help Session
- Center for Scientific Computation Summer Workshop — Week-long, full-day workshop
- Center for Scientific Computation Spring Workshop Series — 14 2-hour workshops
  1. Introduction to ManeFrame II (M2) 2. Using R on ManeFrame II (M2) 3. Introduction to ManeFrame II (M2) 4. Using SAS on ManeFrame II (M2) 5. Introduction to Jupyter Notebooks 6. Accessing Graphical Applications on ManeFrame II (M2) 7. Introduction to ManeFrame II (M2) 8. Using the NVIDIA P100 Nodes 9. Advanced Slurm Features 10. Introduction to ManeFrame II (M2) 11. Using the Intel Xeon Phi Nodes 12. Parallel Python on ManeFrame II (M2) 13. Tips for Automating Computational Workflows
- Mathworks MATLAB Workshop — 3-hour workshop

2017

- Center for Scientific Computation Fall Workshop Series — 10 2-hour workshops
  1. Migrating to ManeFrame II 2. Introduction to ManeFrame II 3. Debugging Python 4. Parallel Python 5. Introduction to Jupyter Notebooks 6. Porting Applications to MICs and GPUs 7. Introduction to ManeFrame II 8. Debugging Parallel Applications with Allinea DDT 9. Profiling Parallel Applications with Allinea MAP 10. Introduction to ManeFrame II
- Center for Scientific Computation Summer Workshop — Week-long, full-day workshop
- Center for Scientific Computation Spring Workshop Series — 13 3-hour workshops
  1. Introduction to Parallel Computing 2. Introduction to Research Programming 3. Introduction to Parallel Programming 4. Introduction to Research Computing 5. Introduction to Vectorization 6. Introduction to Shared-Memory Parallel Programming 7. Introduction to Distributed-Memory Parallel Programming 8. Introduction to Research Computing 9. Introduction to Accelerator Programming 10. OpenMP Deep Dive 11. MPI Deep Dive 12. Introduction to Research Computing 13. CUDA and OpenCL Deep Dive

2016

- Center for Scientific Computation Fall Workshop Series — 9 3-hour workshops
  1. Open Help Session 2. ManeFrame Introduction 3. GPGPU Development on ManeFrame 4. Introduction to Jupyter 5. Open Help Session 6. ManeFrame Introduction 7. Debugging and Profiling Parallel Applications on ManeFrame 8. ManeFrame Introduction 9. Introduction to Build Automation Development Tools
- Center for Scientific Computation Summer Workshop — Week-long, full-day workshop
- Center for Scientific Computation Spring Workshop Series — 7 3-hour workshops
  1. Introduction to Using ManeFrame 2. Introduction to Julia 3. Python in HPC Environment 4. Parallel Programming on ManeFrame 5. GPGPU Programming Overview 6. OpenCL for HPC 7. Using R on ManeFrame

2015

- Center for Scientific Computation Fall Workshop Series — 6 3-hour workshops
  1. Introduction to Using ManeFrame 2. Introduction to Parallel Programming 3. Post-processing Data Using Python 4. Bash Shell Scripting 5. Introduction to C++ MPI Programming 6. Introduction to GPGPU Programming
- Center for Scientific Computation Summer Workshop — Week-long, full-day workshop

2014

- Advanced Python Programming Workshop — Fall 2014
- Advanced CHARMM Workshop — Spring 2014
- CATCO URVA Workshop

2013

- Graduate/Undergraduate Computational Chemistry Laboratory
- LaTeX Workshop — Spring 2013

2012

- Graduate/Undergraduate Computer Aided Drug Design Laboratory
- CATCO Methods Workshop
- CATCO URVA Workshop

2011

- Graduate/Undergraduate Computational Chemistry Laboratory

2010

- Graduate/Undergraduate Computer Aided Drug Design Laboratory
- Undergraduate General Chemistry Laboratory

2009

- Graduate/Undergraduate Computational Chemistry Laboratory

Student Advisement

Undergraduate

- Carter Koehler, Southern Methodist University
  - Describing electron density through machine learning models — August 2018 to Present
  - Super Computing 2018 Student Cluster Competition — January 2018 to May 2018
- Ethan Britt, University of Texas at Dallas — January 2018 to May 2018

  - Super Computing 2018 Student Cluster Competition
- Mauhib Iqbal, University of Texas at Dallas — January 2018 to May 2018
  - Super Computing 2018 Student Cluster Competition
- Boce Lin, Southern Methodist University — January 2018 to May 2018
  - Super Computing 2018 Student Cluster Competition
- Rick Simon, Southern Methodist University — January 2018 to May 2018
  - Super Computing 2018 Student Cluster Competition
- Vyas Nellutla, University of Texas at Dallas — January 2018 to May 2018
  - Super Computing 2018 Student Cluster Competition
- Moez Janmohammad, Southern Methodist University — January 2016 to May 2016
  - Engaged Learning Big iDeas Project
  - ARM Beowulf cluster prototype

University Activities and Committees

- Search committee member for the Southern Methodist University Office of Information Technology Data Science Consultant hire — 2018
- Search committee member for the Southern Methodist University Office of Information Technology HPC Consultant hire — 2018
- Search committee member for the Southern Methodist University Office of Information Technology Senior HPC Systems Administrator hire — 2017
- Member of core group tasked with the planning, design, acquisition, and implementation of Southern Methodist University's ManeFrame II (M2) cluster — 2016 to 2017

Service and Outreach

- SMU Reads Facilitator — Fall 2018
- Led Southern Methodist University and University of Texas at Dallas joint team application to the Super Computing 2018 Student Cluster Competition — Spring 2018
- 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

Merits

Technical Skills

- Programming in Fortran, C, C++, Objective-C, Python, R
- Parallel high performance and scientific programming experience using MPI, OpenMP, Pthreads, CUDA, OpenCL
- Scripting in Bash, CSH, AWK, Perl, sed, Tcl
- Installation and application of quantum chemical and molecular dynamics programs on High Performance Computing (HPC) clusters
- Quantum chemical programs: Gaussian, Q-Chem, GAMESS, CFOUR, Molpro, NWChem, DIRAC, ORCA, GPAW
- Molecular dynamics programs: CHARMM, NAMD, LAMMPS, Amber, MPDyn, GROMACS, OpenMM
- Molecular visualization programs: VMD, Chimera, Avogadro, IQmol, POV-Ray

- 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
- Administration experience in UNIX using Linux (Red Hat and Debian derivatives), macOS, FreeBSD, and Solaris including installation and configuration
- Structured writing and documentation in LaTeX, BibTeX, reStructuredText, Sphinx, MediaWiki, HTML
- Source code revision control using Git, Mercurial, Subversion

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