Robert Kalescky
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Education:

- Bachelor of Science in Chemical Engineering, minors in Mathematics and Chemistry, Texas Tech University 2001-2006
- Master of Science in Chemistry, University of Texas at Dallas, 2007-2009

Research Experience

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

Research Interests

- 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.

Teaching Experience

- Undergraduate General Chemistry Laboratory, Southern Methodist University, 2010-2011
- Graduate/Undergraduate Computer Aided Drug Design Laboratory, Southern Methodist University, 2010
- Graduate/Undergraduate Computational Chemistry Laboratory, Southern Methodist University, 2011

Conference Presentations

- The 235th meeting of the American Chemical Society, New Orleans, United States, 2008, presentation
- The 41st meeting of the Dallas-Fort Worth Local Section of the American Chemistry Society, Dallas, United States, 2008, presentation

Skills

- Computational modeling using: Gaussian, GAMESS, CFOUR, NWChem, NAMD, VMD, MPDyn, Spartan, SYBYL.
- Quantum mechanical calculations using: RHF, UHF, MP2, B3LYP.
- Calculation of: geometry optimization, transition states, reaction paths, potential energy surfaces, spectroscopic information, binding free energies.
- Programming in: C, C++, Objective-C, Fortran, OpenCL, CUDA, BASIC.
- Parallel computing using: UNIX (Linux, Mac OS X, Solaris) on SPARC, Power, AMD, and Intel computer clusters.

Publications

- Ranatunga, R. J. K. U.; Kalescky, R.; Chiu, C.; Nielsen, S. O. Molecular Dynamics Simulations of

Surfactant Functionalized Nanoparticles in the Vicinity of an Oil/Water Interface. Journal of Physical Chemistry C **2010**, 114, 12151-12157.

- Kalescky, R.; Shinoda, W.; Moore, P. B.; Nielsen, S. O. Area per ligand as a function of nanoparticle radius: a theoretical and computer simulation approach. Langmuir : the ACS journal of surfaces and colloids **2009**, 25, 1352-1359.