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Education

2008	Duke University, PhD Chemistry
2001	Southern Methodist University, MS Chemistry
1999	Texas Christian University, BS Chemistry

Professional Experience

2009-Present	Research Staff Scientist, Oak Ridge National Laboratory (ORNL)
2008-2009	Postdoctoral Research Associate, Center for Molecular Biophysics, ORNL

Selected Publications

- Parks, J.M., A. Johs, M. Podar, R. Bridou, R. A. Hurt, S.D. Smith, S.J. Tomanicek, Y. Qian, S.D. Brown, C.C. Brandt, A.V. Palumbo, J.C. Smith, J.D. Wall, D.A. Elias, L. Liang. 2013, The Genetic Basis for Bacterial Mercury Methylation. *Science*. In press
- R. Chaudret, J.M. Parks and W.T. Yang, Pseudobond parameters for QM/MM studies involving nucleosides, nucleotides and their analogs, *J. Chem. Phys.*, In press.
- Riccardi, D., H-B Guo, J.M. Parks, B. Gu, L. Liang, and J.C. Smith, Cluster-Continuum Calculations of Hydration Free Energies of Anions and Group 12 Divalent Cations. *J. Chem. Theory Comput.* 2013, 9, 555-569.
- Tschaplinski, T.J., Standaert, R.F., N.L. Engle, M.Z. Martin, A. K. Sangha, J.M. Parks, J.C. Smith, R. Samuel, N. Jiang, Y. Pu, A.J. Ragauskas, C.Y. Hamilton, C.X. Fu, Z.-Y. Wang, B.H. Davison, R.A. Dixon and J.R. Mielenz, Down-regulation of the caffeic acid O-methyltransferase gene in switchgrass reveals a novel monolignol analog, *Biotechnol. Biofuels*, 2012, 5:71.
- K. Sangha, J. M. Parks, R. F. Standaert, A. Ziebell, M. Davis, and J. C. Smith, Radical Coupling Reactions in Lignin Synthesis: A Density Functional Theory Study, *J. Phys. Chem. B*, 2012, 116, 4760–4768
- Mintz, B.J. and Parks, J.M. Benchmark interaction energies for hydrogen-bonded complexes containing divalent sulfur, *J. Phys. Chem. A*, 116, 1086-1092 (2012).
- Johs, A., Harwood, I.M., Parks, J.M., Nauss, R. Smith, J.C., Liang, L., Miller, S.M. Structural characterization of intramolecular Hg²⁺ transfer between flexibly-linked domains of mercuric ion reductase, *J. Mol. Biol.* 413, 639–656 (2011).
- Brown, S.D., Guss, A.D., Karpinets, T.V., Parks, J.M., Smolin, N., Yang, S., Land, M.L., Klingeman, D.M., Bhandiwad, A., Rodriguez Jr., M., Raman, B., Shao, X., Mielenz, J.R., Smith, J.C., Keller, M. and Lynd, L.R., Mutant alcohol dehydrogenase leads to improved ethanol tolerance in *Clostridium thermocellum*, *Proc. Nat. Acad. Sci.* 108, 13752-13757 (2011).
- Guo, H.-B., Johs, A., Parks, J.M., Olliff, L., Miller, S.M., Summers, A.O., Liang, L., and Smith, J.C., Structure and conformational dynamics of the metalloregulator MerR upon binding of Hg(II), *J. Mol. Biol.*, 398, 555-568 (2010).
- Parks, J.M., Guo, H., Momany, C., Liang, L., Miller, S.M., Summers, A.O. and Smith, J.C., Mechanism of Hg-C protonolysis in the organomercurial lyase MerB, *J. Am. Chem. Soc.*, 131, 13278-13285 (2009).
- Parks, J.M., Hu, H., Rudolph, J. and Yang, W.T., Mechanism of Cdc25b phosphatase with the small molecule substrate p-nitrophenyl phosphate from QM/MM-MFEP calculations, *J. Phys. Chem. B*, 113, 5217-5224 (2009).

- Parks, J.M., Hu, H., Cohen, A.J. and Yang, W.T., A pseudobond parameterization for improved electrostatics in quantum mechanical/molecular mechanical simulations of enzymes, *J. Chem. Phys.*, 129, 154106, (2008).
- Parks, J.M., Kondru, R.K., Hu, H., Beratan, D.N. and Yang, W.T., Hepatitis C virus NS5b polymerase: QM/MM calculations show the important roles of the internal energy in ligand binding, *J. Phys. Chem. B*, 112 (10), 3168–3176, (2008).
- Hu, H., Lu, Z., Parks, J.M., Burger, S.K., and Yang, W.T., QM/MM Minimum Free Energy Path for accurate reaction energetics in solution and enzymes: Iterative optimization on the potential of mean force surface, *J. Chem. Phys.*, 128, 034105, (2008).
- Sohn, J., Parks, J.M., Buhrman, G., Brown, P., Kristjánsdóttir, K., Safi, A., Edelsbrunner, H., Yang, W.T. and Rudolph, J., Experimental validation of the docking orientation of Cdc25 with its Cdk2-CycA protein substrate, *Biochemistry*, 44, 16563-16573 (2005).
- Parks, J.M., Ford, G.P. and Cramer, C.J., Quantum chemical characterization of the reactions of the phenylnitrenium ion with guanine, *J. Org. Chem.*, 66, 8997-9004 (2001).