Ariana Beste

UT Staff
Joint Institute for Computational Sciences
Oak Ridge National Laboratory
(865) 241-3160
bestea@ornl.gov

Education

Philipps-Universität Marburg, Germany	Chemistry	MS, 1999
Philipps-Universität Marburg, Germany	Computer Science	AS, 1999
University of Florida, Gainesville, FL	Chemistry	PhD, 2004

Professional Experience

2007–present	Research Scientist, Joint Institute for Computational Sciences, ORNL
March 2009	Visiting Scientist, Commonwealth Scientific and Industrial Research Organisation, Newcastle, Australia
2004–2007	Postdoctoral Research, Computational Chemical Sciences Group, ORNL
May-July 1999	Visiting Scientist, Universidad de Barcelona, Barcelona, Spain

Professional and Synergistic Activities

2011	Reviewer for NSF International Collaborations in Chemistry Award
2011	Certificate of Appreciation for Review of Manuscripts Submitted to ACS Journals
2010	American Chemical Society, Division of Fuel Chemistry, R. A. Glenn Award

Selected Publications

1. A, Beste and A. C. Buchanan, III (2012). Challenges in the Computation of Rate Constants for Lignin Model Compounds. In H. DaCosta & M. Fan (Eds.), *Rate Constant Calculation for Thermal Reactions: Methods and Applications* (pp. 191-238). Hoboken, New Jersey: John Wiley & Sons, Inc.
2. A. Beste and A. C. Buchanan, III, Kinetic Simulation of the Thermal Degradation of Phenethyl Phenyl Ether, a Model Compound for the β-O-4 Linkage in Lignin, Chem. Phys. Lett. 550 (2012) 19.
3. J. M. Younker, A. Beste, and A. C. Buchanan, III, Computational Study of Bond Dissociation Enthalpies for Lignin Model Compounds: β-5 Arylcoumaran, Chem. Phys. Lett. 545 (2012) 100.
4. J. M. Younker, A. Beste, and A. C. Buchanan, III, Computational Study of Bond Dissociation Enthalpies for Substitued β-O-4 Lignin Model Compounds, ChemPhysChem 12 (2011) 3556.
5. P. Jackson, A. Beste, and M. Attalla, Insights into Amine-Based CO_2 Capture: An ab initio Self-Consistent Reaction Field Investigation, Struct. Chem. 22 (2011) 537.
6. A. Beste and A. C. Buchanan, III, Kinetic Analysis of the Phenyl-Shift Reaction in β-O-4 Lignin Model Compounds: A Computational Study, J. Org. Chem. 76 (2011) 2195.
7. A. Beste, One-Dimensional Anharmonic Oscillator: Quantum versus Classical Vibrational Partition Functions, Chem. Phys. Lett. 493 (2010) 200.

8. A. Beste and A. C. Buchanan, III, Substituent Effects on the Reaction Rates of Hydrogen Abstraction in the Pyrolysis of Phenethyl Phenyl Ethers, Energy & Fuels 24 (2010) 2857.
9. C. H. Skinner, H. W. Kugel, A. L. Roquemore, P. S. Krstic, and A. Beste, Mass Changes in NSTX Surface Layers with Li Conditioning as Measured by Quartz Microbalances, J. Nuc. Mat. 390-391 (2009) 1005.
10. A. Beste and A. C. Buchanan, III, Computational Study of Bond Dissociation Enthalpies for Lignin Model Compounds. Substituent Effects in Phenethyl Phenyl Ethers, J. Org. Chem. 74 (2009) 2837.

Graduate and Postdoctoral Advisors and Advisees

Harrison, R. J. (ORNL), Bartlett, R. J. (UFL), Frenking, G. (Philipps Universität), Younker, Y. M. (ORNL)