

Name: Ariana Beste
Joint Institute for Computational Sciences
University of Tennessee
1 Bethel Valley Rd., Oak Ridge, TN 37831-6211

Position Title: Research Scientist
(865) 241-3160
(865) 241-4811 FAX
bestea@ornl.gov

Education:

University of Florida, Gainesville Ph.D. 2004 Chemistry
Philipps-Universität, Marburg, Germany, M.S. 1999 Chemistry
Philipps-Universität, Marburg, Germany, A.S. 1999 Computer Science

Professional Experience:

2007-present Research Scientist, Joint Institute for Computational Sciences, University of Tennessee, TN
2009 Visiting Scientist, Commonwealth Scientific and Industrial Research Organisation, Australia
2004 – 2007 Postdoctoral Fellow, Computer Science and Mathematics Division, Oak Ridge National Laboratory, TN
1999 Visiting Scientist, Universidad de Barcelona, Spain

Professional Activities, Honors, and Awards:

2016 Reviewer for ACS Petroleum Research Fund
2015 – present PI of NERSC allocation for computational catalysis
2015 – present PI of CNMS project: Computational study of water interactions with ceria nanocubes
2015 – present PI of discretionary allocation on computational resources of the Oak Ridge Leadership Computing Facility
2013, 2014 Reviewer for director's discretionary allocation proposals at the Oak Ridge Leadership Computing Facility
2013 Reviewer for Laboratory Directed Research and Development funds at ORNL
2012 PI of CNMS project: The role of oxygen-carbon phenyl migration in the pyrolysis mechanism of phenethyl phenyl ether (PPE) and α -hydroxy PPE
2011 Certificate of Appreciation for valuable contributions in the peer review of manuscripts submitted to ACS journals
2011 NSF proposal reviewer
2010 – 2012 PI of ASCR/BES project: Prediction of thermodynamic and kinetic properties for lignin model compounds
2010 Richard A. Glenn Award
2009 Committee Chair awarding travel grants: Summer School in Biophysics at ORNL
2008 – present PI of discretionary allocation on computational resources of the National Institute for Computational Sciences
2004 – present Reviewer for ACS and Elsevier journals
2004 Dow Research Award
1999 – 2002 Grinter fellowship
1999 European fellowship from CESC/CEPBA supercomputer centers

Selected Peer-Reviewed Publications: (total 37)

A. Beste, S. H. Overbury, Hydrogen and Methoxy Coadsorption in the Computation of the Catalytic Conversion of Methanol on the Ceria (111) Surface, *Surface Science*, **648**, 242-249 (2016).
J. E. Sutton, A. Beste, S. H. Overbury, Origins and Implications of the Ordering of Oxygen Vacancies and Localized Electrons on Partially Reduced CeO₂(111), *Phys. Rev. B*, **92**, 144105-1 – 7 (2015).
A. Beste, S. H. Overbury, Pathways for Ethanol Dehydrogenation and Dehydration Catalyzed by Ceria (111) and (100) Surfaces, *J. Phys. Chem. C*, **119**, 2447 - 2455 (2015).

- A. Beste, ReaxFF Study of the Oxidation of Lignin Model Compounds for the Most Common Linkages in Softwood in View of Carbon Fiber Production, *J. Phys. Chem. A*, **118**, 803 - 814 (2014).
- J. M. Younker, T. Saito, M. A. Hunt, A. K. Naskar, A. Beste, Pyrolysis Pathways of Sulfonated Polyethylene, an Alternative Carbon Fiber Precursor, *J. Am. Chem. Soc.*, **135**, 6130 - 6141 (2013).
- A. Beste, A. C. Buchanan, III, Computational Investigation of the Pyrolysis Product Selectivity for α -Hydroxy Phenethyl Phenyl Ether and Phenethyl Phenyl Ether: Analysis of Substituent Effects and Reactant Conformer Selection, *J. Phys. Chem. A*, **117**, 3235 - 3242 (2013).
- A. Beste, Á. Vázquez-Mayagoitia, J. V. Ortiz, Direct Δ MBPT(2) Method for Ionization Potentials, Electron Affinities, and Excitation Energies Using Fractional Occupation Numbers, *J. Chem. Phys.*, **138**, 074101-1 - 074101-13 (2013).
- A. Beste, 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.
- A. Beste, A. C. Buchanan, III, Role of Carbon-Carbon Phenyl Migration in the Pyrolysis Mechanism of β -O-4 Lignin Model Compounds: Phenethyl Phenyl Ether and α -Hydroxy Phenethyl Phenyl Ether, *J. Phys. Chem. A*, **116(50)**, 12242-12248 (2012).
- A. Beste, 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**, 19-24 (2012).

Collaborators:

Thomas J. Elder (Auburn), Álvaro Vázquez Mayagoitia (ANL), J. Vincent Ortiz (Auburn)

Graduate and Postdoctoral Advisors:

Gernot Frenking (Philipps-Universität, retired), Rodney J. Bartlett (University of Gainesville), Robert J. Harrison (Stony Brook)

Total Postdoctoral Scholars Advised: 2