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Position Title: Research Scientist
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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:

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 proposals 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 CESCA/CEPBA supercomputer centers

Selected Peer-Reviewed Publications: (total 36)

J. E. Sutton, A. Beste, S. H. Overbury, Origins and Implications of the Ordering of Oxygen Vacancies and Localized Electrons on Partially Reduced CeO_2(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 ΔMBPT(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 Coumpounds: 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).

A. Beste, D. R. Mullins, S. H. Overbury, R. J. Harrison, Adsorption and Dissociation of Methanol on the Fully Oxidized and Partially Reduced (111) Cerium Oxide Surface: Dependence on the Configuration of the Cerium 4f Electrons, Surface Science, **602**, 162 (2008).

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

Thesis Advisor and Postgraduate-Scholar Sponsor (total 2):
Jonathan E. Sutton (ORNL), Jarod M. Younker (DuPont)