

## VITAE OF BILLY WAYNE MCCANN

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### EDUCATION

Postdoctoral Research Associate, 2013-Present  
Ph.D. in Theoretical/Organic Chemistry, 2013  
B.S. in Chemistry/Mathematics (*summa cum laude*), 2008

ORNL, Oak Ridge, TN  
Auburn University, Auburn, AL  
Troy University, Troy, AL

### HONORS

2011-2012 Merriwether Fellow Nominee, (Auburn University)  
2011 Outstanding Poster Presentation, (Conference on Current Trends in Computational Chemistry)  
2008 The Outstanding Undergraduate Student in Chemistry, (Troy University)  
2006 Recognition for Outstanding Achievement in Calculus-Based Physics II (Wallace College)

### PROFESSIONAL SOCIETIES

American Association for the Advancement of Science, 2012-present  
American Chemical Society, 2008-present

### PUBLICATIONS

1. McCann, B. W.; Bryantsev, S. “*de novo* Molecular Design of Neutral Ligands for Efficient Extraction of Rare Earth Elements.” **2015** *Near submission*
2. McCann, B. W.; Acevedo, O. “Benchmarking Continuum Solvent Models for Keto-Enol Tautomerizations” *J. Phys. Chem. A*, **2015** *In Press*
3. McCann, B. W.; Hay, B.; “HostDesigner 3.0: Enhancements via Advanced Molecular Building Algorithms. Project 1.4.2, Task 2.” Internal Report to the United States Department of Energy Critical Materials Institute. **2014** [http://bwayne.sdf.org/documents/CMI\\_Internal\\_Report.pdf](http://bwayne.sdf.org/documents/CMI_Internal_Report.pdf)
4. Allen, C.; McCann, B. W.; Acevedo, O. “Ionic Liquid Effects on Nucleophilic Aromatic Substitution Reactions from QM/MM Simulations” *J. Phys. Chem. B*, **2014**, *119* (3), 743–752  
doi:10.1021/jp504967r

5. McCann, B. W.; Acevedo, O. "Pairwise Alternatives to Ewald Summation for Calculating Long-Range Electrostatics in Ionic Liquids" *J. Chem. Theory Comput.*, **2013**, 9, 944–950 doi:10.1021/ct300961e
6. McCann, B. W.; Song, H.; Kocer, H. B.; Cerkez, I.; Acevedo, O.; Worley, S. D. "Inter- and Intramolecular Mechanisms for Chlorine Rearrangements in Trimethyl-Substituted N – Chlorohydantoins" *J. Phy. Chem. A.* **2012**, 116, 7245-7252 doi:10.1021/jp304610k

## **PRESENTATIONS**

1. Pairwise Alternatives to Ewald Summation for Calculating Long-Ronge Electrostatics in Ionic Liquids. McCann, B.W.; Acevedo, O. *National ACS Conference, New Orleans* **2013**
2. Benchmarking Continuum Solvation Models and Cavities for the Accurate Calculation of Condensed Phase Tautomerization Equilibria. McCann, B.W.; Acevedo, O. *Gorden Research Conference, Mount Snow Resort, Dover, VA*, **2012** (poster)
3. Exploring the Role of Ionic Liquids on Aromatic Nucleophilic Substitution Reactions via QM/MM Simulations. Allen, C.; McCann, B.W.; Acevedo, O. *Southeast Theoretical Chemistry Association Annual Meeting, University of Georgia, Athens, GA*, **2012**. (poster)
4. Solute Cavity Sizes and Solution Phase Protomer Equilibria. McCann, B.W.; Acevedo, O. *Southeast Theoretical Chemistry Association Annual Meeting, University of Georgia, Athens, GA*, **2012**. (poster)
5. Solvation Models and Tautomerism Thermodynamics. McCann, B.W.; Acevedo, O., *Conference on Current Trends in Computational Chemistry, Jackson, MI*, **2011**. Award winning poster presentation.
6. Dynamics of Methyl-substituted Cyclopentanes at Conical Intersections. *Auburn Univerisity*, **2010**

## **SKILLS AND QUALIFICATIONS**

Programming: Python, Fortran  
Scheme, Shell (bash, zsh, csh)

Chemistry Softwares: Gaussian, BOSS, GAMESS, MOPAC  
PCModel, Avagadro, UCSF Chimera  
Tinker, Cambridge Structure Database

Linux computing cluster maintenance

## **SOFTWARE PRODUCTS**

HostDesigner 3.0 – *de novo* Computer-Aided Molecular Design Software Package

## **TEACHING**

Auburn University, Auburn, AL

- Teaching Assistant: CHEM 2071, Organic I Chemistry Lab (2009-2013)
- Teaching Assistant: CHEM 2081, Organic II Chemistry Lab (2009-2013)
- Teaching Assistant: CHEM 1111, General Chemistry Lab (2008-2009)
- Tutoring: Department of Chemistry and Biochemistry (2008-2013)

### **ACTIVITIES AND OUTREACH**

2012 Southeast BEST Robotics Southeast Division Competition – Judge  
2012 AU EXPLORE Chemistry Demonstrator  
2012 Auburn University Division B Regional Science Olympiad Event Supervisor and Judge  
2011 Southeast BEST Robotics Competition – Judge  
2009 AU Science Day Chemistry Demonstrator  
fightmalaria@home participant  
mathematics, physics, and chemistry tutor  
*pro bono* tutoring for in-need students

### **EMPLOYMENT**

2013-present, Postdoctoral Research Associate, Oak Ridge National Lab, TN  
2012-2013, Research Assistant, Auburn University, Auburn, AL  
2008-2012, Teaching Assistant (Organic Chemistry), Auburn University, Auburn, AL  
2006-2008, Waiter, Outback Steakhouse, Dothan, AL  
2005-2006, Laser Technical Specialist, Lasertech Surgical Support Services, Dothan, AL  
2000-2005, Surgical Technician, Southeast Alabama Medical Center, Dothan, AL