10/2009

VITA OF ORLANDO ACEVEDO

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Education

Postdoctoral Associate, 2003-2006:	Yale University, New Haven, CT
Ph.D. in Theoretical/Organic Chemistry, 2003:	Duquesne University, Pittsburgh, PA
B.S. in Chemistry, 1998:	Florida International University, Miami, FL

Employment

2006 - present, Assistant Professor, Department of Chemistry and Biochemistry, Auburn University

2003-2006 Postdoctoral Associate, Yale University. QM/MM simulations and Monte Carlo calculations of organic and enzymatic reactions. Advisor: William L. Jorgensen.

1999-2003 Graduate Student, Duquesne University. Large-scale DFT calculations for catalyst design. Advisor: Jeffrey D. Evanseck.

1996-1998 Research Assistant, Florida International University. Molecular dynamics simulations of non-naturally occurring amino acids situated in short peptides. Advisor: David Chatfield.

Awards and Fellowships

2008 Hewlett-Packard Outstanding Junior Faculty Award, (ACS)
2004 IUPAC Prize for Young Chemists, (IUPAC)
1999-2000 Outstanding Academic Record Fellowship, (University of Miami)

Member or Officer in Professional Societies

American Chemical Society, 1999 - present.
Newsletter Editor (Officer), Computers in Chemistry Division 2003-present
Chair-Elect, Auburn Local Section of the ACS, 2009; Chair 2010
New York Academy of Sciences, 2004 - 2007.

Publications

25. Sheppard, A.N.; Acevedo, O.; "Multidimensional Exploration of Valley-Ridge Inflection Points on Potential Energy Surfaces" *J. Am. Chem. Soc.*, **2009**, *131*, 2530-2540.

24. Sambasivarao, S.V.; Acevedo, O. "Development of OPLS-AA Force Field Parameters for 68 Unique Ionic Liquids" *J. Chem. Theory Comput.*, **2009**, *5*, 1038-1050.
~Featured on the cover (June 2009)

23. Acevedo, O.; Jorgensen, W.L. "Advances in Quantum and Molecular Mechanical (QM/MM) Simulations for Organic and Enzymatic Reactions" *Acc. Chem. Res.*, **2009**, (in press). http://dx.doi.org/10.1021/ar900171c

22. Acevedo, O. "Determination of Local Effects for Chloroaluminate Ionic Liquids on Diels-Alder Reactions" *J. Mol. Graphics and Modell.*, **2009**, 28, 95-101.

21. Acevedo, O. "Role of Water in the Multifaceted Catalytic Antibody 4B2 for Allylic Isomerization and Kemp Elimination Reactions" *J. Phys. Chem. B,* **2009**, (in press).

20. Acevedo, O.; Armacost, K. "Insight into "On Water" Catalysis from QM/MM Simulations" **2009**, (manuscript submitted)

19. Acevedo, O.; Squillacote, M.E.; "A New Solvent-Dependent Mechanism for a Triazolinedione Ene Reaction" *J. Org. Chem.,* **2008**, *73*, 912-922.

18. Akdag, A.; Worley, S.D.; Acevedo, O.; McKee, M.L.; "Mechanism of 5,5-Dimethylhydantoin Chlorination: Monochlorination through a Dichloro Intermediate" *J. Chem. Theory Comput.,* **2007**, *3*, 2282-2289.

17. Acevedo, O.; Jorgensen, W.L.; "Understanding Rate Accelerations for Diels-Alder Reactions in Solution Using Enhanced QM/MM Methodology" *J. Chem. Theory Comput.,* **2007**, 3, 1412-1419.

16. Gunaydin, H.; Acevedo, O.; Jorgensen, W.L.; Houk, K.N..; "Computation of Accurate Barriers for Methyl Transfer Reactions of Sulfonium and Ammonium Salts in Aqueous Solutions" *J. Chem. Theory Comput.,* **2007**, 3, 1028-1035.

15. Acevedo, O.; Jorgensen, W.L.; Evanseck, J.D.; " Elucidation of Rate Variations for a Diels-Alder Reaction in Ionic Liquids from QM/MM Simulations" *J. Chem. Theory Comput.,* **2007**, 3, 132-138.

14. Tubert-Brohman, I.; Acevedo, O.; Jorgensen, W.L.; " Elucidation of Hydrolysis Mechanisms for Fatty Acid Amide Hydrolase and Its Lys142Ala Variant via QM/MM Simulations" *J. Am. Chem. Soc.,* **2006**, *128*, 16904-16913.

13. Acevedo, O.; Jorgensen, W.L.; "Cope Elimination: Elucidation of Solvent Effects from QM/MM Simulations" *J. Am. Chem. Soc.,* **2006**, *128*, 6141-6146.

12. Acevedo, O.; Jorgensen, W.L.; "Medium Effects on the Decarboxylation of a Biotin Model in Pure and Mixed Solvents from QM/MM Simulations" *J. Org. Chem.,* **2006**, *71*, 4896-4902.

11. Acevedo, O.; Jorgensen, W.L.; "Solvent Effects on Organic Reactions from QM/MM Simulations" in *Annual Reports in Computational Chemistry*, Elsevier, (Spellmeyer, Ed.) **2006**, Vol. 2, 263-278.

10. Acevedo, O.; Jorgensen, W.L.; "Influence of Inter- and Intramolecular Hydrogen Bonding on Kemp Decarboxylations from QM/MM Simulations" *J. Am. Chem. Soc.,* **2005**, *127*, 8829-8834.

9. Boger, D.L.; Miyauchi, H.; Du, W.; Hardouin, C.; Fecik, R.A.; Cheng, H.; Hwang, I.; Hedrick, M.P.; Leung, D.; Acevedo, O.; Guimaraes, C.R.W.; Jorgensen, W.L.; Cravatt, B.F.; "Discovery of a Potent, Selective, and Efficacious Class of Reversible α-Ketoheterocycle Inhibitors of Fatty Acid Amide Hydrolase Effective as Analgesics" *J. Med. Chem.*, **2005**, *48*, 1849-1856.

8. Acevedo, O.; Evanseck, J.D.; "Transition Structures and Transition States" in *Computational Medicinal Chemistry for Drug Discovery,* Dekker Inc., New York, **2004**, Chapter 12, 323-344.

7. Acevedo, O.; Jorgensen, W.L.; "Solvent Effects and Mechanism for a Nucleophilic Aromatic Substitution from QM/MM Simulations" *Org. Lett.*, **2004**, *6*, 2881-2884.

6. DeChancie, J.; Acevedo, O.; Evanseck, J.D.; "Density Functional Theory Determination of an Axial Gateway to Explain the Rate and Endo Selectivity Enhancement of Diels-Alder Reactions by Bis(oxazoline)-Cu(II)" *J. Am. Chem. Soc.*, **2004**, *126*, 6043-6047.

5. Loccisano, A.E.; Acevedo, O.; DeChancie, J.; Schulze, B.G.; Evanseck, J.D.; "Enhanced Sampling by Multiple Molecular Dynamics Trajectories: Carbonmonoxy Myoglobin 10 μs A0 → A1-3 Transition from Ten 400 Picosecond Simulations" *J. Mol. Graphics Modell.*, **2004**, *22*, 369-376.

4. Acevedo, O.; Evanseck, J.D.; "The Effect of Solvent on a Lewis Acid Catalyzed Diels-Alder Reaction Using Computed and Experimental Kinetic Isotope Effects" *Org. Lett.*, **2003**, *5*, 649-652.

3. Acevedo, O.; Evanseck, J.D.; "Transition Structure Models of Organic Reactions in Chloroaluminate Ionic Liquids. Cyclopentadiene and methyl acrylate Diels-Alder reaction in acidic and basic melts of 1-ethyl-3-methylimidazolium chloride with aluminum(III) chloride" *ACS Symposium Series*, **2003**, *856 (Ionic Liquids as Green Solvents: Progress and Prospects)*, 174-190.

2. Dick, T.J.; Acevedo, O.; Dalal, P.; Madura, J.D.; Evanseck, J.D.; Mathews, J.P. "Molecular Basis For Carbon Dioxide Sequestration In Coal" *Reprints of Symposia-American Chemical Society, Division of Fuel Chemistry*, **2002**, *47*, 14-16.

1. Acevedo, O.; Schulze, B.G.; Evanseck, J.D.; "The Gates, Swings and Levers of Biomolecular Mechanics" *Phys. Chem. 2000, Proc. Int. Conf. Fundam. Appl. Aspects Phys. Chem. 5th*, **2000**, 264-277.

Invited Presentations

13. "Computational organic and bioorganic chemistry" Auburn University, March **2009**.

12. "Advances in computational biochemistry: Role of water in catalytic antibodies" University of South Alabama, Sept. **2008**.

11. "Advances in computational biochemistry: Role of water in catalytic antibodies" University of Alabama at Birmingham, Sept. **2008**.

10. "Advances in potentials of mean force methodology for organic and biological simulations" Southeastern Theoretical Chemistry Association, University of Alabama, May **2008**.

9. "The chemistry of carbon" Focus the Nation Symposium, Auburn University, Jan. **2008**.

8. "Advances in QM/MM simulations for computational biochemistry" Armstrong Atlantic State University, Nov. **2007**.

7. "Advances in QM/MM simulations for computational biochemistry" Auburn University – Department of Physics, Sept. **2007**.

6. "Computational organic chemistry: Elucidation of solvent effects from water to ionic liquids" Auburn University, Jan. **2006**.

5. "Computational organic chemistry: Elucidation of solvent effects from water to ionic liquids" Grinnell College, Dec. **2005**.

4. "Kemp decarboxylation: The influence of hydrogen bonding" Hobart and William Smith Colleges, Dec. **2005**.

3. "The influence of inter- and intramolecular hydrogen bonding on Kemp decarboxylations from QM/MM simulations" Yale University, April **2005**.

2. "Understanding how ionic liquids influence the Diels-Alder reaction" University of Washington, Seattle, Dec. **2004**.

1. "Understanding how ionic liquids influence the Diels-Alder reaction" Florida State University, Nov. **2004.**

Contributed Presentations

25. (Oral) "Solvent-dependent mechanisms for triazolinedione and singlet oxygen ene reactions from QM/MM simulations" Acevedo, O.*; Book of Abstracts, 238th ACS National Meeting, Washington, D.C. August 16-20, **2009**.

24. (Oral) “Computer Simulations of Steroid Transformation in Ketosteroid Isomerase” Thigpen, C.*; Acevedo, O.; 6th Annual AU CMB Undergraduate Research Symposium, April 6-7, **2009**.

23. (Oral) “Development and validation of OPLS-AA force field parameters for ionic liquid simulations” Acevedo, O.*, Sambasivarao, S.V.; 236th ACS National Meeting, Philadelphia, PA, Aug. **2008**.

22. (Poster) “Systematic development of OPLS-AA force field parameters for ionic liquid simulations” Sambasivarao, S.V.*, Acevedo, O.; 236th ACS National Meeting, Philadelphia, PA, Aug. **2008**.

21. (Poster, invited) “Advances in potentials of mean force methodology for organic and biological simulations” Acevedo, O.;* Book of Abstracts, 235th ACS National Meeting, New Orleans, LA April 6-11, **2008.**

20. (Poster) “Elucidation of the mechanism of hydrolysis by fatty acid hydrolase (FAAH) from QM/MM simulations” Tubert-Brohman, I.;* Acevedo, O.; Jorgensen, W.L.; Fall Meeting of the Swiss Chemical Society 2007, École Polytechnique Fédérale de Lausanne September 12, **2007.**

19. (Oral) “Medium effects on organic reactions featuring elimination mechanisms in pure and mixed solvents from QM/MM simulations” Acevedo, O.;* Book of Abstracts, 233th ACS National Meeting, Chicago, IL March 25-29, **2007.**

18. (Oral) “Theoretical investigation of ionic liquids in the catalysis of the Diels-Alder reaction” Acevedo, O.;* Jorgensen, W.L., Evanseck, J.D.; Book of Abstracts, 231th ACS National Meeting, Atlanta, GA March 26-30, **2006**.

17. (Poster) “Disconnection of maximum stereoelectronic effects from the transition structure” Plumley, J.A.;* Evanseck, J.D.; Acevedo, O.; Book of Abstracts, 231th ACS National Meeting, Atlanta, GA March 26-30, **2006**.

16. (Poster) “Exploring solvent effects and mechanisms for organic reactions using computational methods”, Acevedo, O.;* Jorgensen, W.L.; Book of Abstracts, 230th ACS National Meeting, Washington, D.C. August 28-September 1, **2005**.

15. (Poster) “Understanding how external influences impact reaction rates and selectivity” Acevedo, O.;* Jorgensen, W.L.; Book of Abstracts, 228th ACS National Meeting, Philadelphia, PA, August 22-26, **2004**.

14. (Oral) “Advances in QM/MM simulations for organic reactions in solution” Jorgensen, W.L.;* Guimaraes, C.R.W.; Acevedo, O.; Book of Abstracts, 227th ACS National Meeting, Anaheim, CA, March 28-April 1, **2004**.

13. (Oral) “Understanding how ionic liquids impact the Diels-Alder reaction: An ab initio, semiempirical and QM/MM approach” Acevedo, O.; Evanseck, J.D.;* Book of Abstracts, 227th ACS National Meeting, Anaheim, CA, March 28-April 1, **2004**.

12. (Oral) “Density functional investigation of ionic liquid cation-anion ratios in the catalysis of Diels-Alder reactions” Acevedo, O.;* Evanseck, J.D.; Book of Abstracts, 226th ACS National Meeting, New York, NY, September 7-11, **2003**.

11. (Poster) “Varying Lewis acidity in ionic liquids with new force field parameters” Acevedo, O.;* Evanseck, J.D.; Book of Abstracts, 226th ACS National Meeting, New York, NY, September 7-11, **2003**.

10. (Poster) “Synthesis Density functional theory study of the influences of the N-1-butylpyridinium and chloroaluminate ratios upon the rates and endo/exo selectivity of the Diels-Alder reaction” Waligorski, A.M.;* Acevedo, O.; Evanseck, J.D.; Book of Abstracts, 226th ACS National Meeting, New York, NY, September 7-11, **2003**.

9. (Poster) “Principles of chemical reactivity in ionic liquids using quantum and molecular mechanics” Acevedo, O.;* Evanseck, J.D.; Book of Abstracts, 225th ACS National Meeting, New Orleans, LA, March 22-27, **2003**.

8. (Poster) “A density-functional exploration of copper(II) aqua ion and chiral bis(oxazoline) copper(II) Diels-Alder transition structures” Dechancie, J.;* Acevedo, O.; Evanseck, J.D.; Book of Abstracts, 225th ACS National Meeting, New Orleans, LA, March 22-27, **2003**.

7. (Oral) “Perturbing the Diels-Alder transition structure” Acevedo, O.;* Evanseck, J.D.; Book of Abstracts, 224th ACS National Meeting, Boston, MA, August 18-22, **2002**.

6. (Oral) “Theoretical assessment on how ionic liquids influence chemical reactivity and stereoselectivity of organic reactions” Evanseck, J.D.;* Acevedo, O.; Book of Abstracts, 224th ACS National Meeting, Boston, MA, August 18-22, **2002**.

5. (Poster) “Transition structures and ionic cages in ionic liquids” Acevedo, O.;* Evanseck, J.D.; Book of Abstracts, 224th ACS National Meeting, Boston, MA, August 18-22, **2002**.

4. (Poster) “Models of bis(oxazoline)-Cu(II) complexes upon Diels-Alder reactions” Dechancie, J.;* Acevedo, O.; Evanseck, J.D.; Book of Abstracts, 224th ACS National Meeting, Boston, MA, August 18-22, **2002**.

3. (Oral) “Novel transition structure interactions in boron Lewis acid catalyzed Diels-Alder reactions” Acevedo, O.;* Kong, S.; Evanseck, J.D.; Book of Abstracts, 223th ACS National Meeting, Orlando, FL, April 7-11 **2002**.

2. (Poster) “Molecular details of how ionic liquids influence chemical reactivity and stereoselectivity” Acevedo, O.;* Evanseck, J.D.; Book of Abstracts, 223th ACS National Meeting, Orlando, FL, April 7-11 **2002**.

1. (Poster) “Theoretical assessment of catalytic and stereoselective influence of bis(oxazoline)-Cu(II) complexes upon Diels-Alder reactions” Dechancie, J.;* Acevedo, O.; Evanseck, J.D.; Book of Abstracts, 223th ACS National Meeting, Orlando, FL, April 7-11 **2002**.

Current Co-workers
Somisetti V. Sambasivarao (Ph.D. 2011)
Caley Allen (Ph.D. 2012)
Kira Aramacost (Ph.D. 2012)
Billy McCann (Ph.D. 2012)
Christen Thigpen (B.S. 2010)
Benjamin Moltz (B.S. 2010)
Samantha Essick (B.S. 2011)

Past Co-workers
April Sheppard (B.S. 2008)

Courses Taught
Fall 06, 07, 08, and 09 semesters, CHEM 5280/6280 Computational Chemistry
Spring 08, CHEM 2070, Organic Chemistry I
Spring 09, CHEM 2080, Organic Chemistry II