

Brooke Michelle Otten

brookeotten@my.unt.edu

Ph.D. Graduate Student | University of North Texas
| Department of Chemistry



EDUCATION

Ph.D. in Chemistry Inorganic Chemistry Division (Current GPA: 3.7)

University of North Texas, Denton, Texas, U.S.A.

Advisor: Dr. Mohammad A. Omary

B.Sc. in Chemistry with a Minor in Mathematics (ACS Certified) (GPA: 3.0) May 2015

University of North Texas, Denton, Texas, U.S.A.

Advisor: Dr. Thomas R. Cundari

TEACHING EXPERIENCE

Graduate Teaching Assistant:

August 2014 - Present

- Computational Chemistry Instructional Lab
 - Assists students in use of computational chemistry software
 - Teaches students how use research software (including citing software, Scifinder)
- Training Undergraduate Chemist
 - Teaching students to use computational chemistry methods to solve real world problems
 - Organizing projects for students to work through
 - Monitoring progress of students through meetings and progress reports
 - Helping students to produce presentations on research results
- Laboratory Teaching Assistant
 - Teaching weekly general chemistry (I and II), organic chemistry (I and II) and inorganic laboratory courses

- Preparing and teaching weekly pre-lab lectures
- Enforcing chemical lab safety requirements
- Mentoring students on correct laboratory procedures and data analysis

Undergraduate Tutoring Experience

August 2011 – May 2014

- Chemistry
 - Taught general chemistry (I and II) and organic chemistry (I) concepts
 - Planned and taught weekly lectures
 - Developed and administered weekly checkpoint quizzes
- Math
 - Taught college algebra, linear algebra and calculus (I) concepts
 - Developed weekly lectures
 - Assisted with homework and reviews

RESEARCH EXPERIENCE

Graduate Research Assistant

August 2014 - Present

- Analyzing d^{10} - d^{10} bonding characteristics in bridged Pt/Pd/Ni complexes
- Determining the effects of counter ion substitution on the spin orbit couple splitting of triplet excited states of Gold(I)-phosphine complexes via computational and experimental methods.
- Predicting structures and excitation and emission energies of Copper(I) complexes through a computational study.
- Analyzing the energetics of oxidative addition and reductive elimination to coinage metal cyclic trimers as well as dimers of trimers, via computational methods to help guide experimental chemist in producing catalyst for hydrogen gas production.
- Using computational chemistry to help guide the synthesis of anti-corrosion materials to be used as coatings.
- Determined degree of bonding between Gold(I) and Copper(I) centers through use of Morse potential plots and bond order analysis calculations.
- Assessed the acceptor behavior of fluorinated coinage metal trimers with sulfur containing donors through the use of binding energies.
- Studied the effects of solvent and halo-ligands on emission energies of Gold(I)phosphine complexes through a photoluminescence study.
- Studied photoluminescence and redox behavior of Platinum containing complexes through a computational study to help explain experimental phenomena.
- Completed a study on the molar volume of Pt(II) complex and various quenchers to help explain experimental phenomena.

REU Participant

June 2014 – August 2014

- Investigated extent of excited state distortions in neutral coinage metalphosphine complexes through the use of DFT methods.
- Reproduced synthesis and photoluminescence studies of Gold(I)-phosphine complexes through the use of schlenck line technique.

Undergraduate Research Assistant

August 2010 – December 2013

- Investigated the ground state and transition state structures of multiple azide complexes to help explain reactivity with a Nickel(II) complex.
- Analyzed the effects of different oxygen atom delivery reagents on oxy-atom insertion to Rh(III) and Pt(III) hydrocarbyl complexes through use of DFT methods.
- Analyzed energetics and transition states of oxy-insertion into Rhenium(III) methyl bonds using biological catalyst (Flavin) through a computational study using DFT methods.

COMPUTATIONAL EXPERIENCE WITH

- Gaussian09
- ADF
- VASP
- Quantum-Espresso
- GAMESS

SOFTWARE

- Gaussview
- Chemcraft
- Origin
- Cambridge Database
- PTIFELIX32
- Microsoft Office Package (Word, Excel, Powerpoint)
- Familiar with Python

TECHNICAL SKILLS

- Schlenck line technique
- Photoluminescence
- Infrared Spectroscopy
- UV-Vis Spectroscopy

AWARDS

- Marshall Education Award (May 2015)
- George Vaughan Memorial Award (May 2016)
- Graduate Seminar Day – 2nd place (April 2017)

PUBLICATIONS

7. Sinha, P.; **Otten, B.M.**; Wang, X.; Omary, M.A. "Colossal Luminescence Rigidochromic Shifts in Cationic and Neutral Three-Coordinate Au(I)Phosphine Complexes Via Control of Photoinduced Jahn-Teller Distortion" *J. Am. Chem. Soc.*, **In preparation.**
6. Smith, J.B.; **Otten, B.**; Derry, P.J.; Browning, C.; Sandridge, J.; Satumtira, N.T.; Zilaie, M.; Payne, J.; Nuti, R.; Omary, M.A.; Smucker, B.W. "Luminescent, redox-active (dithiolato)bis(imine)platinum(II) divergent complexes with exchangeable imine ligands: An experimental/computational study versus their (diamine)(dithiolato)platinum(II) convergent congeners" *Inorg. Chem.*, **In preparation.**
5. Dharmawardana, M.; Ghimire, M.; Fallah, H.; **Otten, B.**; Kaipa, U.; Arimilli, B.; McCandless, G.; Cundari, T.; Omary, M.; Gassensmith, J. "Colossal Anisotropic Expansion and Thermochromism in a Single Crystal Organic Semiconductor: A Structural, Photophysical and, Computational Study" **In preparation.**
4. Galassi, R.; Ghimire, M.M.; **Otten, B. M.**; Ricci, S.; McDouglad Jr., R.N.; Almotawa, R.; Alhmoud, D.; Ivy, J. F.; Rawashdeh, A.-M.; Nesterov, V.N.; Reinheimer, E.W.; Daniels, L. M.; Burini, A.; Omary, M.A. "21st Century Alchemy: Cupriphication of Gold to Sensitize d¹⁰-d¹⁰ Metal-Metal Bonds and Near-Unity Phosphorescence Quantum Yields" *Proc. Nat. Acad. Sci.*, **Manuscript Accepted. FIRST AUTHOR CONTRIBUTION.**
3. **Otten, B.**; Figg, T.; Cundari, T. "The Curious Case of Mesityl Azide and Its Reactivity With bpyNiEt₂" *Inorg. Chem.*, **2014**, 53(21), 11633-11639.
2. Webb, J.; Figg, T.; **Otten, B.**; Cundari, T.; Gunnoe, T.; Sabat, M. "Pt(III) and Rh(III) Hydrocarbyl Complexes Bearing Coordinated Oxygen Atom Delivery Reagents" *Eur. J. Inorg. Chem.*, **2013**, 2013(25), 4515-4525.
1. Pouy, M.; Milczek, E.; Figg, T.; **Otten, B.**; Prince, B.; Gunnoe, T.; Cundari, T.; Groves, J. "Flavin-Catalyzed Insertion of Oxygen Into Rhenium-Methyl Bonds", *J. Am. Chem. Soc.* **2012**, 134(31), 1290-1293.

PRESENTATIONS

9. **Otten, B.M.**; Omary, M.A. To Be or Not to Be: d¹⁰-d¹⁰ Bonding in Heterometallic Complexes. *50th Annual Meeting-in-Miniature*, Texas Christian University, Fort Worth, Texas, April 29th, 2017.
8. **Otten, B.M.**; Bagus, P.S.; Omary, M.A. Giant Texas-Sized Spin-Orbit Splitting in Au(I)-Phosphine Complexes. *72nd Annual Southwest Regional Meeting*, Galveston, TX, United States, November 10-13, 2016, 673.
7. **Otten, B.M.**; Ghimire, M.M.; Tekarli, S.M.; Omary, M.A. Computational/Experimental Investigation of Oxidative Addition and Photoinduced Reductive Elimination in Coinage Metal Cyclotrimers and

- Aggregates Thereof: Toward Next-Generation Classes of Photocatalysts. *72nd Annual Southwest Regional Meeting*, Galveston, TX, United States, November 10-13, 2016, 136.
6. Omary, M.A.; **Otten, B.M.**; Bagus, P.S. Giant Spin-Orbit Splitting in Au(I)Phosphine Complexes. *252nd ACS National Meeting & Exposition*, Philadelphia, PA, United States, August 21-25, 2016, INOR-539.
 5. **Otten, B.M.**; Ghimire, M.M.; Tekarli, S.M.; Omary, M.A. Computational/Experimental Investigation of Oxidative Addition and Photoinduced Reductive Elimination in Coinage Metal Cyclotrimers and Aggregates Thereof: Toward Next-Generation Classes of Photocatalysts. *252nd ACS National Meeting & Exposition*, Philadelphia, PA, United States, August 21-25, 2016, INOR-664.
 4. **Otten, B.M.**; Tekarli, S.M.; Omary, M.A. Calculating" Next-Generation Solar Photocatalysts: Computational Investigation of the Oxidative Addition and Photoinduced Reductive Elimination of Halogens to Coinage Metal Cyclotrimers. *49th Annual Meeting-In-Miniature*, Texas Woman's University Denton, Texas, April 23rd, 2016.
 3. **Otten, B.M.**; Omary, M.A. Giant Spin-Orbit Coupling Microstate Splitting of the Lowest Triplet in Phosphorescent Au(I) Complexes. Philipps Universität Marburg, Germany, May 18-22, 2015.
 2. **Otten, B.M.**; Ghimire, M.M.; Omary, M.A. Excited State Distortion of Gold, Silver and Copper (I)-Phosphine Complexes. *NSF-REU Poster Presentation*, Denton, Texas, August 7th, 2014.
 1. **Otten, B.M.**; Omary, M.A. Excited State Distortions in Neutral Au(I)-Phosphine Complexes. *NSF-REU Presentation*, Denton, Texas, United States, July 2nd, 2014.

Extracurricular Activities

- Social Officer (2016-Present)
- Graduate Recruitment weekend (2017)
- Graduate Recruitment weekend (2016)
- Graduate Recruitment weekend (2015)
- Volunteer Science Fair Judge (2015)