

Dr. Bruce M. Prince, Ph.D.

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Research and Teaching Experience:

My research focuses on designing novel organometallic catalysts using density functional theory (DFT) and *ab initio* methods, I have used the correlation consistent Composite Approach (ccCA) developed at UNT. Additionally, I have investigated hydrogen tunneling via nuclear-electronic orbital-MCSCF (NEO-MCSCF) approaches. Specific applications I have investigated include: α -olefin hydroarylation, styrene catalysis, C-H bond activation and functionalization, olefin epoxidation, oxidation of metal-alkyl complexes, C-N bond coupling, and CO₂ fixation. Presently, I am a Visiting Assistant Professor at Texas Southern University (TSU) in the Chemistry Department working with the students and continuing my research. In addition, I am currently teaching physical chemistry, the upper division and graduate level inorganic courses.

Educational Background:

1. Ph.D., Inorganic Chemistry; University of North Texas, Denton, Texas 2014
Concentration in Inorganic Chemistry with a specialization in Computational Chemistry
Adviser and mentor: Dr. Thomas R. Cundari
2. BS, Inorganic Chemistry California State University, Bakersfield, CA 1996

Title of Ph.D. Dissertation: The Mechanisms of Methane C-H Activation and Oxy-Insertion via Small Transition Metal Complexes: A DFT Computational Investigation

Academic Experience:

1. Teaching and Research Texas Southern University 2014-present
 2. Ph.D. Research Assistant University of North Texas 2010-2014
 3. Ph.D. Teaching Assistant (TA) University of North Texas 2009-2010
1. Prepared lectures for science majors: General, Physical, Inorganic and Advance Inorganic chemistry (TSU).
 2. Graded all class lab coursework while teaching the labs at the University of North Texas (UNT).
 3. Promote positive student learning outcomes through engaging active teaching.
 4. Maintained regularly scheduled office hours to provide assistance to students in chemistry while working as a lab instructor at the University of North Texas (UNT).
 5. Trained in student recruiting with the lead recruiter at the UNT Chemistry Department.

Collaborators Since 2009

1. T. Brent Gunnoe (University of Virginia)
2. Tom R. Cundari (University of North Texas)
3. C. J. Tymczak (Texas Southern University)
4. Olayinka Olatunji-Ojo (University of California, Berkeley)
5. Mahmoud A. Saleh (Texas Southern University)

Peer-Reviewed Publications:

1. Co^I-Me Catalyzed Carboxylation of Carbon Dioxide Plus Methane into Acetic Acid by Tuning the Catalytic Activities with Small Substituents- **Prince, B. M.**; (Manuscript in Progress)
2. DFT Study of the Reaction of a Two-Coordinate Iron(II) Dialkyl Complex with Molecular Oxygen; **Prince, B. M.**, Cundari, T. R.; Tymczak, C. J.; *J. Phys. Chem. A*, **2013**, 117, 9245–9251 DOI: [10.1021/jp5082438](https://doi.org/10.1021/jp5082438)
3. Oxy-functionalization of Group 9 and 10 Transition Metal Methyl Ligands: Use of Pyridine-based Hemi-labile Ligands; **Prince, B. M.**, Gunnoe, T. B., Cundari, T. R.; *Dalton Trans.*, **2014**, **2014**, 43, 7608-7614 DOI: [10.1039/C4DT00371C](https://doi.org/10.1039/C4DT00371C)
4. Pt^{II} Catalyzed Hydrophenylation of α -Olefins: Variation of Linear: Branched Products as a Function of Ligand Donor Ability; McKeown, B. A., **Prince, B. M.**, Ramiro, Z., Gunnoe, T. B., Cundari, T. R.; *ACS Catal.*, **2014**, 4, 1607-1615 DOI: [10.1021/cs400988w](https://doi.org/10.1021/cs400988w)
5. Methane C—H Bond Activation by “Naked” Alkali Metal Imidyl and Alkaline Earth Metal Imide Complexes. The Role of Ligand Spin and Nucleophilicity; **Prince, B. M.**, Cundari, T. R., *J. Phys. Chem. A*, **2013** 117, 9245-9251 DOI: [10.1021/JP404951E](https://doi.org/10.1021/JP404951E)
6. Flavin-catalyzed Insertion of Oxygen into Rhenium-Methyl Bonds; Pouy, M. J., Milczek, E. M., Gunnoe, T. B., Figg, T. M., **Prince, B. M.**, Otten, B. M., Cundari, T. R., *J. Am. Chem. Soc.* **2012**, 134,12920-12923, (communication); DOI: [10.1021/JA3054139](https://doi.org/10.1021/JA3054139)
7. C—H Bond Activation of Methane by Pt^{II}-N-Heterocyclic Carbene Complexes. The Importance of Having the Ligands in the Right Place at the Right Time; **Prince, B. M.**, Cundari, T. R., *Organometallics*, **2012**, 31, 1042–1048., DOI: [10.1021/OM201114D](https://doi.org/10.1021/OM201114D)
8. DFT Study of the Reactivity of Methane and Dioxygen with d¹⁰-L₂M Complexes; Cundari, T. R., **Prince, B. M.**, *J. Organomet. Chem.* **2011**, 696, 3982-3986., DOI: [10.1016/j.jorganchem.2011.06.015](https://doi.org/10.1016/j.jorganchem.2011.06.015)
9. Redox Insertion into Metal-Carbon Bonds. A Computational Study of Pt⁰ and Pt^{II} N-Heterocyclic Carbene Complexes; **Prince, B. M.**, Cundari, T. R.; (Manuscript is Completed – awaiting internal review by CCHF experimental collaborators).

Invited Journal Review:

1. “N-Acetylserotonin and 6-Hydroxymelatonin against Oxidative Stress: Implications for the Overall Protection Exerted by Melatonin” Álvarez-Diduk, R.; *J. Phys. Chem. A.* (2015)
2. “Mechanism of Action of Sulforaphane as a Superoxide Radical Anion and Hydrogen Peroxide Scavenger by Double Hydrogen Transfer: A Model for Iron Superoxide Dismutase”; Prasad, A. K., Mishra, P.C.; *J. Phys. Chem. A.* (2015)
3. “Sulfur Dioxide Activation: A Theoretical Investigation into S=O Dual Bond Cleavage by Three-Coordinate Molybdenum(III) Complexes”; Robinson, R Jr., Ariafard, A., Khadem, K. A., Stranger, R., and Yates, B. F.; *Inorg Chem.* (2014)

Oral Presentations:

1. “A DFT Study of Oxy-Insertion into Metal-Carbon Bonds via Organometallic Baeyer-Villiger and Oxo Transformations” 240th ACS National Meeting, Boston, August 22-26, 2010.
2. “Redox & Non-Redox Carbon-Oxygen Formation” University of North Texas (UNT), Denton, November 21st 2010.
3. “Redox vs. Non-Redox Oxy Insertion into Metal Carbon Bonds” Center for Catalytic Hydrocarbon Functionalization (CCHF 2011), Charlottesville, June 1-3, 2011.

4. "Redox vs. Non-Redox Oxy Insertion into Metal Carbon Bonds" Southwest Theoretical Chemistry Conference (SWTCC 2011), Lubbock, TX, October 21-23, 2011.
5. "Methane-to-Methanol (MTM) Catalysis" Center for Catalytic Hydrocarbon Functionalization (CCHF 2012), Charlottesville, May 30-June 1, 2012.
6. "Methane-to-Methanol (MTM) and Olefin Hydroarylation Catalysis" University of North Texas (UNT), Denton, October, 24th, 2012.
7. "DFT Potential Energy Surface Studies of Cationic bipy-Pt(II) Complexes for the Formation of Alkyl Arenes by α -Olefin Hydroarylation Catalysis" 245th ACS National Meeting, New Orleans, April 7-11, 2013.
8. "DFT and Experimental Investigation of Pt(II) α -olefin Hydroarylation" University of North Texas (UNT), Denton, June 20th, 2013.
9. "Platinum Mediated C-H and C-O Bond Formation" Texas Southern University (TSU), Houston, August 9th, 2013.
10. "The Mechanisms of Methane C-H Activation and Oxy-insertion via DFT Computational Investigation" Texas Southern University (TSU), Houston, February 27th, 2014.
11. "The Medley of Transition Metals via Computational Chemistry" Texas Southern University (TSU), Houston, September 26th, 2014
12. "Mechanisms of Methane C-H Activation and Oxy-insertion Via Transition Metal Complexes: DFT Investigations" Prairie View A&M University (PVAMU), Prairie View, July 09th, 2015

Research Expertise Includes:

1. Designing advanced catalysts for functionalization of hydrocarbon gases into liquid fuels.
2. Designing advanced catalysts for carboxylation of CO₂ fixation with alkyl and aryl substrates
3. Designing novel catalysts to directly convert arenes and olefins into alkyl-arenes via C-C and C-H bond activation.
4. Modeling of hydrogen transfer reactions by means of nuclear-electronic orbital (NEO) methods.
5. One-step methane-to-methanol (MTM) partial oxidation catalysis.
6. DFT and *ab initio* investigations of the aerobic oxidation of organometallics.
7. The correlation consistent Composite Approach (ccCA) modeling of s-block metal complexes.
8. Excited states of [L_nM-NH₂] complexes.

Academic and Professional Honors and Awards:

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| 1. | Graduate Assistantship Tuition Scholarship (GATS) | 2012-2013 |
| 2. | Academic Achievement Scholarship | 2009-2012 |
| 3. | Competitive Scholarship Waiver | 2009-2012 |
| 4. | Graduate Student Support Travel Grant | 2011 |
| 5. | DOE Scholarship Grant Award | 2011 |
| 6. | USC (University Scholarship Committee) Scholarship for Continuing Students | 2010-2011 |

Employment History:

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|----|---|------------------|--------------|
| 1. | Texas Southern University
Visiting Assistant Professor
Physical Chemistry | TSU, Houston, TX | 2015-present |
| 2. | Texas Southern University | TSU, Houston, TX | 2015-present |

Visiting Assistant Professor
General Chemistry

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| 3. | Texas Southern University
Adjunct Professor
Inorganic Chemistry | TSU, Houston, TX | 2014-2015 |
| 4. | Texas Southern University
Post-doctoral Research Fellow
Funded by CREST
Working with Prof. Christopher J. Tymczak | TSU, Houston, TX | 2014-2015 |
| 5. | University of North Texas
Graduate RA (CCHF)
Graduate Teaching Assistant (TA) | UNT, Denton, TX | 2009-2014 |
| 6. | Prince Agency, Inc.
Owner, Allstate Insurance and Financial Services | Bellingham, WA | 2004-2009 |
| 7. | Shell Refinery
Petrochemical Technician/Lab Manager | Anacortes, WA | 1992-2004 |
| 8. | Flasher Oil
Petrochemical Technician | Carson, CA | 1984-1992 |

Mentoring/Advising:

Duration	Student Name	Classification	Type	Project/Thesis Dissertation Supervised
2014-Present	Miles Sewell	Undergraduate Student	Mentoring	

Volunteer Work:

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| 1. | ACS
ACS Graduate & Postdoctoral Scholars Reception | New Orleans | 2013 |
| 2. | University of North Texas (UNT)
Graduate Recruitment | Lubbock | 2011 |

Skills:

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| 1. | Microsoft Word, Excel and PowerPoint | 6. | Chemcraft |
| 2. | Gaussian 09/03 | 7. | GAMESS |
| 3. | GaussView 3.0/5.0 | 8. | Refworks |
| 4. | CSD (Cambridge Structural Database) | 9. | SciFinder |
| 5. | ChemDraw | | |

Professional Membership:

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| 1. | Center for Research in Complex Networks (CRCN) | 2014-present |
| 2. | American Chemical Society | 2009-present |
| 3. | Center for Advanced Scientific Computing and Modeling (CASCaM) | 2009-2014 |
| 4. | University of North Texas, Department of Chemistry (Team Cundari) | 2009-2014 |

Professional Leadership Skills:

1. “Proposal Development Workshop for the National Science Foundation (NSF)’s Major Research Instrumentation (MRI) Program and Research Initiation Awards (RIA) Strand of the Historically Black Colleges and Universities-Undergraduate Program (HBCU-UP)” Quality Education For Minorities (QEM) Network, Linthicum Heights, MD, August 14-15, 2015