

# Dr. Bruce M. Prince, Ph.D.

## Teaching and Research Experience:

My research focuses on the analysis of organometallic chemistry, catalysis design with transition metals and main group chemistry via density functional theory (DFT), and ab initio methods, I have used the correlation consistent Composite Approach (ccCA) developed at UNT. The main goal of my basic researches is to understand what controls C-H bond activation, from a fundamental perspective. Presently, I am an Assistant Professor at Texas Southern University (TSU) in the Chemistry Department working with students and continuing my research. In addition, I am currently teaching physical chemistry and graduate level advance physical chemistry courses. Here my research ranges from Earth-abundant chemistry, the investigation of methane C-H activation by first-row late transition metal non-innocent complexes. Previous work completed during my PhD studies and Postdoctoral Fellowship predominately looked at N-heterocyclic carbene and carbon donor ligands coordinated to late transition metals, and their related chemistry. This lead to the investigation of an improved and accurate DFT methodology for computing catalytic mechanisms, specifically Fe-catalyzed, Group 9 and 10 - catalyzed oxy-insertion methyl migration pathway. Additionally, I have investigated hydrogen tunneling via nuclear-electronic orbital-MCSCF (NEO-MCSCF) approaches. Specific applications I have investigated include:  $\alpha$ -olefin hydroarylation, styrene catalysis, C-H bond activation and functionalization, olefin epoxidation, oxidation of metal-alkyl complexes, C-N bond coupling, non-innocent complex, and CO<sub>2</sub> fixation, I have used computational chemistry to model and understand interesting structures. Other structural interests include conformational analysis using the Cambridge Structural Database (CSD), which now used by my physical chemistry students.

## 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. Assistant Professor of Chemistry Texas Southern University 2016-Present
2. Visiting Assistant Professor Texas Southern University 2014-2016
3. Ph.D. Research Assistant University of North Texas 2010-2014
4. Ph.D. Teaching Assistant (TA) University of North Texas 2009-2010
5. Prepared lectures for science majors: General, Physical, Inorganic and Advance Inorganic and Physical chemistry courses (TSU).
6. Teach undergraduate labs at the University of North Texas (UNT).
7. Promote positive student learning outcomes through engaging active teaching.
8. Maintained regularly scheduled office hours to provide assistance to students in chemistry while investigating reaction pathways *via* computational chemistry at both UNT and TSU.
9. Trained in student recruiting with the lead recruiter at the UNT Chemistry Department.

## Graduate Faculty Status:

Spring 2015-present

## **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. Methane C-H Activation by 3d-Metal Amide/Aminyl Complexes. The Role of the Non-Innocent Ligand – **Prince, B.M.**; Cundari, T.R. (in progress)
2. Substituent Effects of Carbon Dioxide Fixation: A DFT Investigation into the O=C=O bond Cleavage by Three-Coordinate Cobalt (I) Complex Followed by Methane C-H activation-**Prince, B. M.**; (Manuscript Completed)
3. 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*, **2014**, 118, 11056-11061 DOI: [10.1021/jp5082438](https://doi.org/10.1021/jp5082438)
4. 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)
5. Pt<sup>II</sup> Catalyzed Hydrophenylation of  $\alpha$ -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)
6. 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)
7. 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)
8. C—H Bond Activation of Methane by Pt<sup>II</sup>-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)
9. DFT Study of the Reactivity of Methane and Dioxygen with d<sup>10</sup>-L<sub>2</sub>M 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)
10. Redox Insertion into Metal-Carbon Bonds. A Computational Study of Pt<sup>0</sup> and Pt<sup>II</sup> 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” 240<sup>th</sup> ACS National Meeting, Boston, August 22-26, 2010.
2. “Redox & Non-Redox Carbon-Oxygen Formation” University of North Texas (UNT), Denton, November 21<sup>st</sup> 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, 24<sup>th</sup>, 2012.
7. “DFT Potential Energy Surface Studies of Cationic bipy-Pt(II) Complexes for the Formation of Alkyl Arenes by  $\alpha$ -Olefin Hydroarylation Catalysis” 245<sup>th</sup> ACS National Meeting, New Orleans, April 7-11, 2013.
8. “DFT and Experimental Investigation of Pt(II)  $\alpha$ -olefin Hydroarylation” University of North Texas (UNT), Denton, June 20<sup>th</sup>, 2013.
9. “Platinum Mediated C-H and C-O Bond Formation” Texas Southern University (TSU), Houston, August 9<sup>th</sup>, 2013.
10. “The Mechanisms of Methane C-H Activation and Oxy-insertion via DFT Computational Investigation” Texas Southern University (TSU), Houston, February 27<sup>th</sup>, 2014.
11. “The Medley of Transition Metals via Computational Chemistry” Texas Southern University (TSU), Houston, September 26<sup>th</sup>, 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 09<sup>th</sup>, 2015

### **Research Expertise Includes:**

1. Designing advanced catalysts for functionalization of hydrocarbon gases into liquid fuels.
2. Designing advanced catalysts for carboxylation of CO<sub>2</sub> 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<sub>n</sub>M-NH<sub>2</sub>] 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<br>Associate Professor<br>Physical Chemistry and General Chemistry                               | TSU, Houston, TX | 2016-Present |
| 2. | Texas Southern University<br>Visiting Assistant Professor<br>Physical Chemistry  | TSU, Houston, TX | 2014-2016    |
| 3. | Texas Southern University<br>Adjunct Professor<br>Inorganic Chemistry  | TSU, Houston, TX | 2014-2015    |
| 4. | Texas Southern University<br>Post-doctoral Research Fellow<br>Funded by CREST<br>Working with Prof. Christopher J. Tymczak | TSU, Houston, TX | 2014-2015    |
| 5. | University of North Texas<br>Graduate RA (CCHF)<br>Graduate Teaching Assistant (TA)  | UNT, Denton, TX  | 2009-2014    |
| 6. | Prince Agency, Inc.<br>Owner, Allstate Insurance and Financial Services  | Bellingham, WA   | 2004-2009    |
| 7. | Shell Refinery<br>Petrochemical Technician/Lab Manager   | Anacortes, WA    | 1992-2004    |
| 8. | Flasher Oil<br>Petrochemical Technician  | Carson, CA       | 1984-1992    |

## **Mentoring/Advising:**

Duration	Student Name	Classification	Type	Project/Thesis Dissertation
2014 - 2015	Miles Sewell	Undergraduate Student	Mentoring	Supervised

## **Volunteer Work:**

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

## Graduate Recruitment

### **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. CCDC       |
| 5. ChemDraw                             | 10. SciFinder |

### **Professional Membership:**

- |  |              |
|--|--------------|
| 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

### **References:**

**Dr. Thomas R. Cundari**, Regents Professor  
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