Dr. Bruce M. Prince
bruce.prince@tsu.edu

Teaching and Research Experience:

My research focuses on teaching and designing novel organometallic catalysts using density functional theory (DFT) and *ab initio methods.* I have also used the correlation consistent Composite Approach (ccCA) developed at University of North Texas (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, small alkyl species and ammine C-H and N-H activations, oxy-insertion and methyl migration, olefin epoxidation, oxidation of metal-alkyl complexes, C-N bond coupling, aminyl radical complex, and CO_2 fixation. Presently, I am a Tenure Track Assistant Professor at Texas Southern University (TSU) in the Chemistry Department working with students and continuing my research. In addition, currently I am teaching general chemistry for science majores, physical chemistry and graduate level advance physical chemistry courses.

Educational Background:

1. Postdoc Fellow in Computational Chemistry, Texas Southern University, Houston, TX: 1/2014-1/2015
2. 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
3. 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. Tenure Track Assistant Professor Texas Southern University 2016-Present
2. Visiting Assistant Professor Texas Southern University 2014-2016
3. Post-doctoral Research Fellow Texas Southern University 2014-2015
4. Ph.D. Research Assistant University of North Texas 2010-2014
5. Ph.D. Teaching Assistant (TA) University of North Texas 2009-2010
6. Prepared lectures for science majors: general, physical, inorganic and advance inorganic and physical chemistry courses (TSU).
7. Teach undergraduate labs at the University of North Texas (UNT) and TSU.
8. Promote positive student learning outcomes through engaging active teaching.
9. Maintained regularly scheduled office hours to aid students in chemistry while investigating reaction pathways *via* computational chemistry at both UNT and TSU.
10. Recruiting students with the lead recruiter at the UNT Chemistry Department.

Teaching Experience:

CHEM 131	Online General Chemistry I for Science Majors	2 courses
CHEM 132	Online General Chemistry II for Science Majors	2 courses
CHEM 131	General Chemistry I for Science Majors	7 courses
CHEM 132	General Chemistry II for Science Majors	6 courses
CHEM 411	Physical Chemistry Lab I	7 courses
CHEM 431	Physical Chemistry Lecture I	7 courses
CHEM 412	Physical Chemistry Lab II	5 courses
CHEM 432	Physical Chemistry Lecture II	5 courses
CHEM 450	Inorganic Chemistry	1 course
CHEM 531	Advanced Inorganic Chemistry	1 course
CHEM 623	Chemistry Special Topics	1 course
CHEM 635	Advance Physical Chemistry	1 course
CHEM 861	Individual Research for Master's Thesis	3 courses

Directed Students Learning:

Thesis Committee Chair, Chemistry.	2017 - Present
Thesis Committee Member, Chemistry.	2016 - 2018

Graduate Faculty Status:

Advisor	2015 - Present

Invited Summer Research:

Michigan State University (Dr. Angela Wilson)	Summer 2018

Collaborators Since 2009:

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

Peer-Reviewed Publications:

1. A DFT Computational Study of Methane C−H and Ammine N−H Activation by Group 9 Pyrrolyl Complexes – **Prince, B. M.,** *Comput. Theor. Chem*, **2019**, 1162, 112503., DOI https://doi.org/10.1016/j.comptc.2019.112503
2. Computational Study of Methane C−H Activation by Earth-Abundant Metal-Amide/Aminyl Complexes **Prince, B. M.,** Cundari, T,R.; *Organometallics*, **2017**, *36*, 3987-3994**.,** DOI**:** 10.1021/acs.organomet.7b00600
3. A DFT Investigation of Substituent Effects on Carbon Dioxide Fixation: by a Low-Coordinate Cobalt (I) Complex– **Prince, B.M.,** *Comput. Theor. Chem*, **2017**, 1122, 1-8., DOI: org/10.1016/j.comptc.2017.10.014
4. 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
5. 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**, 43, 7608-7614 DOI: 10.1039/C4DT00371C

6. 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
7. 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
8. 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
9. 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
10. DFT Study of the Reactivity of Methane and Dioxygen with d^{10}-L_2M Complexes; Cundari, T. R., **Prince**, **B. M.,** *J. Organomet. Chem.* **2011**, *696*, 3982-3986., DOI: 10.1016/j.jorganchem.2011.06.015
11. Redox Insertion into Metal-Carbon Bonds. A Computational Study of Pt^0 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 Reviews:

1. "Zinc complexes with 1,2-disubstituted benzimidazole ligands: experimental and theoretical studies in the catalytic cycloaddition of CO_2 with epoxides: Jorge Luiz Sônego Milani, Werberson de Almeida Bezerra, Ana Karoline Silva Mendanha Valdo, Felipe Terra Martins, Lilian Tatiane Ferreira de Melo Camargo, Valter Henrique Carvalho-Silva, Sailer Santos dos Santos, Danielle Cangussu, Rafael Pavão das Chagasa; *Polyhedron*, (**2019**)
2. "A DFT perspective for the complexation of actinyl with graphdiyne"; Raza ullah shah Bacha, Ting-Ting Lin, Jun Yao, Li, Li-Chun Xuan, and Qing-Jiang Pan; *Comput. Theor. Chem*, (**2019**)
3. "Gas-phase Activation of Methane with $PtOH^{+}$"; Shaoli Liu*, Jianbo Cheng, Qingzhong Li, Wenzuo Li*; *Comput. Theor. Chem*, (**2018**)
4. "A theoretical study on 5,6-dihydroxy-2-methyl-1-benzofuran-3-carboxylate derivatives" Karimia, P.; Ahmara, H.; Makaremb, S. *Comput. Theor. Chem*, (**2017**)
5. "N-Acetylserotonin and 6-Hydroxymelatonin against Oxidative Stress: Implications for the Overall Protection Exerted by Melatonin"; Álvarez-Diduk, R.; *J. Phys. Chem. A.* **(2015)**
6. "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)**
7. "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)**

Invited Grant Proposal Reviews:

1. "CAREER: Catalysts in Motion - Ab Initio Molecular Dynamics Simulations in Gold Homogeneous Catalysis"; Siebert, M. R.; CHE - Chemical Catalysis; NSF 17-537; DUNS# 076255876; NSF PROPOSAL NUMBER 1752695; **(2017)**
2. "Theoretical Study of the Strongly Correlated Electronic Structure and Energetics of the Surface Layer in Transition Metal Oxides from First-Principles DFT-DMFT Calculations"; Park, H.; ACS PRF; 58204-DNI5; **(2017)**

3. "Collaborative Research: All C-Atom Quaternary Centers - Integrating Computation and Experiment"; Atesin, T.; Tius, M; CHE - Chemical Synthesis; PD 09-6878; DUNS# 069444511; NSF PROPOSAL NUMBER 1664982; **(2016)**

Oral Presentations:

1. "DFT investigation of Methane (CH_4) and Carbon Dioxide (CO_2) to Acetic Acid." Texas Southern University (TSU), Houston, September 27, 2018.
2. "DFT investigation of Methane (CH_4) and Carbon Dioxide (CO_2) to Acetic Acid" NOBCChE 45 Annual Conference, Orlando, Florida, September 17-20, 2018.
3. "An *in-Silico* Study of Methane C−H Activation by Earth-Abundant Metal-Amide/Aminyl Complexes" NOBCChE 44 Annual Conference, Minneapolis MN, October 30 to November 2, 2017.
4. "A DFT Investigation of Substituent Effects on Carbon Dioxide Fixation: by a Low-Coordinate Cobalt (I) Complex." Texas Southern University (TSU), Houston, April 10, 2017
5. "The C-H Bond Activation by TR-Metals from a Fundamental Perspective." Texas Southern University (TSU), Houston, February 2, 2017.
6. "The C-H Bond Activation by TR-Metals from a Fundamental Perspective." Texas Southern University (TSU), Houston, February 2, 2017.
7. "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, 2015.
8. "The Medley of Transition Metals via Computational Chemistry" Texas Southern University (TSU), Houston, September 26, 2014.
9. "The Mechanisms of Methane C-H Activation and Oxy-insertion via DFT Computational Investigation" Texas Southern University (TSU), Houston, February 27, 2014.
10. "Platinum Mediated C-H and C-O Bond Formation" Texas Southern University (TSU), Houston, August 9th, 2013.
11. "DFT and Experimental Investigation of Pt (II) σ-olefin Hydroarylation" University of North Texas (UNT), Houston, Texas, June 20, 2013.
12. "DFT Potential Energy Surface Studies of Cationic bipy-Pt (II) Complexes for the Formation of Alkyl Arenes by α-Olefin Hydroarylation Catalysis" 245 ACS National Meeting, New Orleans, April 7-11, 2013.
13. "Methane-to-Methanol (MTM) and Olefin Hydroarylation Catalysis" University of North Texas (UNT), Denton, October 24, 2012.
14. "Methane-to-Methanol (MTM) Catalysis" Center for Catalytic Hydrocarbon Functionalization (CCHF 2012), Charlottesville, May 30-June 1, 2012.
15. "Redox vs. Non-Redox Oxy Insertion into Metal Carbon Bonds" Southwest Theoretical Chemistry Conference (SWTCC 2011), Lubbock, TX, October 21-23, 2011.
16. "Redox vs. Non-Redox Oxy Insertion into Metal Carbon Bonds" Center for Catalytic Hydrocarbon Functionalization (CCHF 2011), Charlottesville, June 1-3, 2011.
17. "Redox & Non-Redox Carbon-Oxygen Formation" University of North Texas (UNT), Denton, November 21st, 2010.
18. "A DFT Study of Oxy-Insertion into Metal-Carbon Bonds via Organometallic Baeyer-Villiger and Oxo Transformations" 240 ACS National Meeting, Boston, August 22-26, 2010.

Research Expertise Includes:

1. Designing advanced catalysts for functionalization of small hydrocarbon gases into liquid fuels.
2. Designing advanced catalysts for carboxylation of CO_2 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 and two-step methane-to-methanol (MTM) partial oxidation catalysis.

6. DFT and a*b initio* investigations of the aerobic oxidation of organometallic complexes.
7. The correlation consistent Composite Approach (ccCA) modeling of s-block metal complexes.
8. Amide/aminyl excited states of [L_nM-NH_2] complexes.

Academic and Professional Honors and Awards:

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

Contracts, Grants, Sponsored Research, Pending Support:

1. *Prince, B.M*. (Principal), "A Computational DFT Study of Methane C−H and Ammine N−H Activations by Fe, Co and Ni κ^3-CNC Ligand Complexes," Sponsored by Spencer Foundation, Private, $48,680, *Pending* (2019)
2. *Prince, B.*M. (Principal), Planning and Initiation of the TSU Center for Computational Catalysis Research (**3CR**)," Sponsored by Texas Southern University (TSU), State, $3,500 *Funded* (2017-2018)
3. *Prince, B.M*. (Co-Principal), "Automobile Emission and Air Quality in Greater Houston, Texas: Assessment and Improvement," Sponsored by Center for Complex Networks (CREST) National Science Foundation (NSF), Federal, $5,000,000, *Pending* (2018)
4. *Prince, B.M*. (Principal), "CAREER: Alkaloids Transition Metal Catalysis via C-C plus C-N Insertion with H-H bond Activation Mechanisms to Physostigmine," Sponsored by National Science Foundation (NSF), Federal, $485,920 *Unfunded* (2018)
5. *Prince, B.M.* (Principal), "Excellence in Research: Transition Metal Catalysis via H-H Activation Followed With C-C and C-N Insertion, A Very Simple Mechanism to Desoxynoreseroline," Sponsored by National Science Foundation (NSF), Federal, $369,420 *Unfunded* (2018)
6. *Prince, B.M.* (Principal), "Methane C-H Activation by Earth-Abundant Amide and Aminyl Metal Complexes. The Role of the Non-Innocent Ligand," Sponsored by The Welch Foundation, $112,284 *Unfunded* (2018)
7. *Prince, B.M.* (Principal), "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," Sponsored by The Petroleum Research Fund New Directions Proposal (ACS PFR), $110,000 *Unfunded* (2017)
8. *Prince, B.M.* (Principal), "Methane C-H Activation by Earth-Abundant Aminyl Metal Complexes. The Role of the Non-Innocent Ligand," Sponsored by The Welch Foundation, $110,000 *Unfunded* (2016)

Employment History:

1.	Texas Southern University Assistant Professor of Chemistry Physical Chemistry and General Chemistry	TSU, Houston, TX	2014-Present
2.	Texas Southern University Visiting Assistant Professor Physical Chemistry	TSU, Houston, TX	2014-2016
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:

Year	*Student Name*	*Classification*	*Type*	*Research Type*
2018	Mariel Gonda	High School Graduate	Mentoring	ACS Seed
2018	Timothy Osazuwa	High School Graduate	Mentoring	ACS Seed
2018	Duke Ogega	Graduate Student	Mentoring	Advised
2017	Tavia Fitzpatrick	Undergraduate Student	Mentoring	L-SAMP
2017	Aaron Taylor	Undergraduate Student	Mentoring	L-SAMP
2017	Heaven Banks	High School Student	Mentoring	ACS Seed
2017	Adesuwa Ehioghae	High School Student	Mentoring	ACS Seed
2014	Miles Sewell	Undergraduate Student	Mentoring	Advised

University Service - Committee:

1.	Curriculum Planning and Evaluation	2019 - Present
2.	Committee Chair, Graduate Research Committee	2017 - Present
3.	Graduate School Grievance Committee	2017 - Present
4.	College Grade Appeal Committee	2016 - Present
5.	Committee Member, University Honors Day Convocation	2017 - 2018
6.	Reinstatement Committee	2017 - 2019

External Service - Committee:

1.	NOBCChE Executive Board	2019 - Present
2.	World Harvest Outreach (WHO) SDA Church Board	2017 - Present

Volunteer Work:

1.	NOBCChE	2017, 2018
2.	ACS: ACS Graduate & Postdoctoral Scholars Reception	2013
3.	University of North Texas (UNT): Graduate Recruitment	2011

Skills:

1. Microsoft Word, Excel and PowerPoint
2. Gaussian 09/16
3. GaussView 3.0/5.0
4. CSD (Cambridge Structural Database)
5. ChemDraw
6. Research
7. Teaching
8. Chemcraft
9. Amber 16
10. GAMESS
11. Refworks
12. SciFinder

Professional Membership:

1.	NOBCChE	2014-Present
2.	Center for Catalysis Computational Research (3CR)	2017-Present
3.	ACS - American Chemical Society	2009-Present
4.	Center for Research in Complex Networks (CRCN)	2014-2017
5.	Center for Advanced Scientific Computing and Modeling (CASCaM)	2009-2014
6.	University of North Texas, Department of Chemistry (Team Cundari)	2009-2014

Professional Leadership Skills:

1. "Proposal Development Workshop for the National Science Foundation (NSF) 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.

2. 2018 NSF-CHE Early Career Investigator Workshop, March 26-27, 2018 at the Embassy Suites Alexandria, Virginia.