

## CHARLES EDWIN WEBSTER, PH.D.

Department of Chemistry, Mississippi State University, Mississippi State University Mississippi State, MS 39762 |  
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### EXPERIENCE

#### Mississippi State University, Mississippi State, MS

Associate Department Head 2018 – present  
Professor 2016 – present  
Associate Professor 2014 – 2016

#### The University of Alabama, Tuscaloosa, AL

Adjunct Professor 2016 – present

#### The University of Memphis, Memphis, TN

Adjunct Professor 2014 – present  
Associate Professor 2010 – 2014  
Assistant Professor 2005 – 2010

#### Zhengzhou University, Zhengzhou, P. R. China

Visiting Professor 2007 – 2010

#### Texas A&M University, College Station, TX

Assistant Research Scientist 2004 – 2005  
Lecturer in Department of Chemistry 2002 – 2003  
Post Doctoral Research Associate 1999 – 2004

#### University of Florida, Gainesville, FL

Post Doctoral Research Associate 1999  
Research Assistant 1996 – 1999  
Teaching Assistant 1995 – 1996

#### University of West Florida, Pensacola, FL

Research Assistant 1993 – 1995  
Teaching Assistant 1992 – 1995

### EDUCATION

University of Florida, Gainesville, FL

#### Ph.D., Chemistry

May 1999

Dissertation Title: "Modeling Adsorption: Investigating Adsorbate and Adsorbent Properties"

Advisors: Russell S. Drago (deceased), Michael C. Zerner (deceased), and Michael J. Scott  
(current: Associate Vice President at San Francisco State University)

University of West Florida, Pensacola, FL

#### B.S., Chemistry / Biochemistry

May 1995

Advisor: S. P. Tanner (Retired)

### AWARDS

Benjamin F. Hilburn Faculty Leadership Program 2016-2017  
MSU College of Arts and Sciences Research Award 2016  
National Science Foundation Career Award 2009  
Presentation at 17th SWTCC 2000  
Catalysis Conference Research Award in memory of Dr. Russell S. Drago 1997  
Department of Chemistry Teaching Award, University of Florida 1995 – 1996  
Merck Award in Chemistry 1995

## POSITIONS HELD

*Organometallics*

<b>Editorial Advisory Board</b> American Chemical Society, Student Affiliates Chapter	<b>2016 – present</b>
<b>President</b> National Honor Society, Student Affiliates Chapter	<b>1994 – 1995</b>
<b>President</b> Florida Junior Academy of Science, Student Affiliates Chapter	<b>1990 – 1991</b>
<b>President</b>	<b>1989 – 1991</b>

## PROFESSIONAL MEMBERSHIPS

American Chemical Society	
Division of Inorganic Chemistry	1997 – present
Division of Physical Chemistry	1997 – 2002
Sigma Xi	2003 – present
Student Affiliates Chapter, American Chemical Society at the University of West Florida	1992 – 1995

## GRANTS AND FUNDING RECEIVED

National Science Foundation PFI-TT 1827686 "Optimizing Next-Generation Materials for Organic Light Emitting Diode (OLED) Applications", \$199,989, 2018-2019

National Science Foundation CHE 1800201 "Carbon Dioxide Reduction Using Earth Abundant Metals and Proton Responsive Pyridinol Based Pincer Ligands", \$115,566, 2018-2021

National Science Foundation CAREER CHE 1543490: "Theoretical Studies on Phosphoryl Transfer Enzymes: Transition-State Analogues and Catalysis", \$342,878, 2015-2017; transfer of CHE 0955723

National Science Foundation OIA 1539035: "RII Track-2 FEC: Feeding and Powering the World - Capturing Sunlight to Split Water and Generate Fertilizer and Fuels", \$6,000,000, 2015-2019

TN-SCORE Research Experiences for Undergraduates (REU) Program (sub-contract), \$56,053, 2014-2015, Funding is provided by NSF EPS-1004083

Probing Chemistry Project (Mathematics and Science Partnership Program), Tennessee Department of Education, \$263,796, 2013

MEMVIZ: Visualization System for Teaching Enhancements and Research, FedEx Institute of Technology, \$80,000, 2013

MEMVIZ: Visualization System for Teaching Enhancements and Research, The University of Memphis Technology Access Fee, \$20,000, 2013

MEMVIZ: Visualization System for Teaching Enhancements and Research, The University of Memphis Information Technology Division, \$20,000, 2013

Development of catalysts, FedEx Institute of Technology, \$85,000, 2012-2013

National Science Foundation CHE 1156738: "Research Experience for Undergraduates Site: University of Memphis Interdisciplinary Research in Chemistry", \$270,000, 2012-2015

National Science Foundation CAREER CHE 0955723: "Theoretical Studies on Phosphoryl Transfer Enzymes: Transition-State Analogues and Catalysis", \$650,000, 2010-2015; transferred

National Science Foundation CHE 0911528: "Ultrafast dynamics, mechanism, and linkage isomerization of photosensitive organometallic manganese and chromium complexes", \$390,000, 2009-2012

National Science Foundation CHE 0851880: "Research Experience for Undergraduates Site: Collaborative Chemistry Research at the University of Memphis", \$220,300, 2009-2012

Faculty Research Grant, The University of Memphis, Summer 2007

ConocoPhillips Contract: "Computational screening of small molecules", \$56,964, 2007

ATMI Contract: "Molecular Dimensions for Adsorptives", \$3,000, 2006

Graduate Student Katherine Leigh, American Chemical Society Division of Inorganic Chemistry Travel Award

Undergraduate Student Angelique Greene, NSF REU Chemistry Leadership Group Travel Award

Graduate Student Kristie Ruddick, NASA Harriett G. Jenkins Pre-doctoral Fellowship, \$114,000

Graduate Student Kristie Ruddick, American Chemical Society Women Chemists Committee Travel Award sponsored by Eli Lilly & Company

Graduate Student Kristie Ruddick, American Chemical Society Division of Inorganic Chemistry Travel Award

## PUBLICATIONS [94 PEER-REVIEWED PUBLICATIONS (OUT 257 TOTAL)]

1. P. Wang, G. Liang, C. E. Webster, X. Zhao "Structure-Functional Analysis of Hydrogen Production Catalyzed by Molecular Cobalt Complexes with Pentadentate Ligands in Aqueous Solutions" *Eur J Inorg Chem*, **2020**, 2020, 3534-3547.  
**Front Cover Art:** <https://chemistry-europe.onlinelibrary.wiley.com/doi/full/10.1002/ejic.202000821>
2. A. Obi, J. Walley, N. C. Frey, O. Wong, D. Dickie, C. E. Webster, R. J. Gilliard, Jr. "Tris(Carbene)-Stabilization of Monomeric Magnesium Cations: A Neutral, Non-tethered Ligand Approach" *Organometallics*, **2020**, accepted.
3. H. Shirley, M. T. Figgins, C. M. Boudreaux, N. P. Liyanage, R. W. Lamb, C. E. Webster, E. T. Papish, J. H. Delcamp "Impact of the Dissolved Anion on the Electrocatalytic Reduction of CO<sub>2</sub> to CO with Ruthenium CNC Pincer Complexes" *ChemCatChem*, **2020**, *12*, 4879-4885.
4. S. Das, D. Nugegoda, F. Qu, C. M. Boudreaux, P. E. Burrow, M. T. Figgins, R. W. Lamb, C. E. Webster, J. H. Delcamp, E. T. Papish "Structure Function Relationships in Ruthenium Carbon Dioxide Reduction Catalysts with CNC Pincers Containing Donor Groups" *Eur J Inorg Chem*, **2020**, 2709-2717.
5. K. E. Krantz, S. L. Weisflog, N. C. Frey, W. Yang, D. A. Dickie, C. E. Webster, R. J. Gilliard, Jr. "Planar, Stair-Stepped, and Twisted: Modulating Structure and Photophysics in Pyrene- and Benzene-Fused N-Heterocyclic Boranes" *Chem Eur J*, **2020**, *26*, 10072-10082.
6. P. Wang, G. Liang, N. Smith, K. Hill, B. Donnadieu, C. E. Webster, X. Zhao "Enhanced Hydrogen Evolution in Neutral Water Catalyzed by a Cobalt Complex with a Softer Polypyridyl Ligand" *Angew Chem Int Ed*, **2020**, *59*, 12694-12697.
7. K. E. Krantz, S. L. Weisflog, W. Yang, D. A. Dickie, N. C. Frey, C. E. Webster, R. J. Gilliard, Jr. "Extremely twisted and bent pyrene-fused N-heterocyclic germylenes" *Chem Commun*, **2019**, *55*, 14954-14957.
8. P. R. Fontenot, B. Shan, B. Wang, S. Simpson, G. Raganathan, A. F. Greene, A. Obanda, L. A. Hunt, N. I. Hammer, C. E. Webster, J. T. Mague, R. H. Schmehl, J. P. Donahue. "Photocatalytic H<sub>2</sub>-Evolution by Homogeneous Molybdenum Sulfide Clusters Supported by Dithiocarbamate Ligands" *Inorg Chem*, **2019**, *58*, 16458-16474.
9. S. Das, R. R. Rodrigues, R. W. Lamb, F. Qu, E. Reinheimer, C. M. Boudreaux, C. E. Webster, J. H. Delcamp, E. T. Papish "Highly Active Ruthenium CNC Pincer Photocatalysts for Visible-Light-Driven Carbon Dioxide Reduction" *Inorg Chem*, **2019**, *58*, 8012-8020.
10. P. Wang, G. Liang, C. L. Boyd, C. E. Webster, X. Zhao "Catalytic H<sub>2</sub> Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand" *Eur J Inorg Chem*, **2019**, 2134-2139.
11. Y. O. Wong, L. A. Freeman, A. D. Agakidou, D. A. Dickie, C. E. Webster, R. J. Gilliard, Jr. "Two Carbenes versus One in Magnesium Chemistry: Synthesis of Terminal Dihalide, Dialkyl, and Grignard Reagents" *Organometallics*, **2019**, *38*, 688-696.
12. G. K. Kosgei, D. Breen, R. W. Lamb, M. Y. Livshits, L. A. Crandall, C. J. Ziegler, C. E. Webster, J. J. Rack. "Controlling Photoisomerization Reactivity Through Single Functional Group Substitutions in Ruthenium Phosphine Sulfoxide Complexes" *J Am Chem Soc*, **2018**, *140*, 9819-9822.
13. P. Wang, G. Liang, M. R. Reddy, M. Long, K. Driskill, C. Lyons, B. Donnadieu, J. C. Bollinger, C. E. Webster, X. Zhao. "Electronic and Steric Tuning of Catalytic H<sub>2</sub> Evolution by Cobalt Complexes with Pentadentate Polypyridyl-Amine Ligands" *J Am Chem Soc*, **2018**, *140*, 29, 9219-9229.
14. J. A. Denny, R. W. Lamb, S. W. Reilly, B. Donnadieu, C. E. Webster, T. K. Hollis. "Investigation of Metallation/Transmetallation Reactions to Synthesize a Series of CCC-NHC Co Pincer Complexes and Their X-ray Structures" *Polyhedron*, **2018**, *151*, 568-574.
15. H. H. C. Lakmal, J. X. Xu, X. Xu, B. Ahmed, C. Fong, D. J. Szalda, K. Ramig, A. Sygula, C. E. Webster, D. Zhang, X. Cui. "Synthesis of C-unsaturated 1,2-Diazetidines and their Ring-opening Reactions via Selective N-N Bond Cleavage" *J Org Chem*, **2018**, *83*, 9497-9503.
16. G. Liang, T. K. Hollis, C. E. Webster. "Computational Analysis of the Intramolecular Oxidative Amination of an Alkene Catalyzed by the Extreme  $\pi$ -loading N-Heterocyclic Carbene Pincer Tantalum(V) Bis(imido) Complex" *Organometallics*, **2018**, *37*, 1671-1681.
17. A. Huckaba, H. Shirley, R. W. Lamb, S. Guertin, S. Autry, H. Cheema, K. Talukdar, T. Jones, J. Jurss, A. Dass, N. I. Hammer, R. Schmehl, C. E. Webster, J. H. Delcamp. "A Mononuclear Tungsten Photocatalyst for H<sub>2</sub> Production" *ACS Catal*, **2018**, *8*, 4838-4847.
18. D. B. Burks, S. Davis, R. W. Lamb, X. Liu, R. R. Rodrigues, N. P. Liyanage, Y. Sun, C. E. Webster, J. H. Delcamp, E. T. Papish. "Nickel(II) pincer complexes demonstrate that the remote substituent controls catalytic carbon dioxide reduction" *Chem Commun*, **2018**, *54*, 3819-3822.
19. G. Liang, C. E. Webster. "The Missing Agostomer in the Fluxionality of Cyclohexenylmanganese Tricarbonyl" *J Organometallic Chem*, **2018**, *864*, 128-135.
20. C. J. Saint-Louis, R. N. Shavnore, C. D. C. McClinton, J. A. Wilson, L. L. Magill, B. M. Brown, R. W. Lamb, C. E. Webster, A. K. Schrock, M. T. Huggins. "Synthesis, computational, and spectroscopic analysis of tunable highly fluorescent BN-1,2-azaborine derivatives containing the N-BOH moiety" *Org Biomol Chem*, **2017**, *15*, 10172-10183.
21. G. Liang, C. E. Webster. "Phosphoramidate Hydrolysis Catalyzed by Human Histidine Triad Nucleotide Binding Protein 1 (hHint1): A Cluster-model DFT Computational Study" *Org Biomol Chem*, **2017**, *15*, 8661-8668.
22. T. R. Helgert, C. E. Webster, T. K. Hollis, H. U. Valle, P. Hillesheim, A. G. Oliver. "Free Methylidyne? CCC-NHC Tantalum Bis(imido) Reactivity: Protonation, Rearrangement to a Mixed Unsymmetrical CCC-N-Heterocyclic Carbene/N-Heterocyclic Dicarbene (CCC-NHC-NHDC) Pincer Tantalum Bis(imido) Complex" *Inorg Chim Acta*, **2017**, *469*, 164-172.
23. G. Liang, N. J. DeYonker, X. Zhao, C. E. Webster. "Prediction of the Reduction Potential in Transition-Metal Containing Complexes: How Expensive? For What Accuracy?" *J Comput Chem*, **2017**, *38*, 2430-2438.
24. J. D. Cope, N. P. Liyanage, P. J. Kelley, J. A. Denny, E. J. Valente, C. E. Webster, J. H. Delcamp, T. K. Hollis. "Electrocatalytic Reduction of CO<sub>2</sub> with CCC-NHC Pincer Nickel Complexes" *Chem Commun*, **2017**, *53*, 9442-9445.
25. J. D. Cope, J. A. Denny, R. W. Lamb, L. E. McNamara, N. I. Hammer, C. E. Webster, T. K. Hollis "Synthesis, characterization, photophysics, and a ligand rearrangement of CCC-NHC pincer nickel complexes: Colors, polymorphs, emission, and Raman spectra" *J Organometallic Chem*, **2017**, *845*, 258-265.

26. S. Siek, D. B. Burks, D. L. Gerlach, G. Liang, J. M. Tesh, C. R. Thompson, F. Qu, J. E. Shankwitz, R. M. Vasquez, N. Chambers, G. J. Szulczewski, D. B. Grotjahn, C. E. Webster, and E. T. Papish "Iridium and Ruthenium Complexes of N-Heterocyclic Carbene- and Pyridinol-Derived Chelates as Catalysts for Aqueous Carbon Dioxide Hydrogenation and Formic Acid Dehydrogenation: The Role of the Alkali Metal" *Organometallics*, **2017**, 36, 1091-1106.
27. R. L. Letterman, N. J. DeYonker, T. J. Burkey, C. E. Webster "Calibrating Reaction Enthalpies: the Use of Density Functional Theory and the Correlation Consistent Composite Approach in the Design of Photochromic Materials" *J Phys Chem A*, **2016**, 120, 9982-9997.
28. C. J. Saint-Louis, L. L. Magill, J. A. Wilson, A. R. Schroeder, S. E. Harrell, N. S. Jackson, J. A. Trindell, S. Kim, A. R. Fisch, L. Munro, V. J. Catalano, C. E. Webster, P. P. Vaughan, K. S. Molek, A. K. Schrock, and M. T. Huggins "The Synthesis and Characterization of Highly Fluorescent Polycyclic Azaborine Chromophores" *J Organic Chem*, **2016**, 81, 10955-10963.
29. **Editor's Choice Cover Article:** T. R. Helgert, X. Zhang, H. K. Box, J. A. Denny, H. U. Valle, A. G. Oliver, G. Akurathi, C. E. Webster, and T. K. Hollis "Extreme  $\pi$ -Loading as a Design Element for Accessing Imido Ligand Reactivity. A CCC-NHC Pincer Tantalum Bis(imido) Complex: Synthesis, Characterization, and Catalytic Oxidative Amination of Alkenes" *Organometallics*, **2016**, 35, 3452-3460.
30. T. K. Hollis, T. R. Helgert, C. E. Webster, H. U. Valle, A. G. Oliver "CCC-NHC Tantalum Bis(imido) Reactivity: Protonation or Rearrangement to a Mixed, Unsymmetrical CCC-N-Heterocyclic Carbene/N-Heterocyclic Dicarbene (CCC-NHC-NHDC) Pincer Tantalum Bis(imido) Complex" *POLYMAT Contributions*, **2016**, 1, 120-126.
31. W. D. Clark, K. N. Leigh, C. E. Webster, and T. K. Hollis "Experimental and Computational Studies of the Mechanisms of Hydroamination/Cyclisation of Unactivated  $\alpha,\omega$ -Amino-alkenes with CCC-NHC Pincer Zr Complexes" *Aust. J. Chem.*, **2016**, 69, 573-582.
32. S. W. Reilly, C. E. Webster, T. K. Hollis, H. U. Valle. "Transmetalation from CCC-NHC pincer Zr complexes in the synthesis of air-stable CCC-NHC pincer Co(III) complexes and initial hydroboration trials" *Dalton Trans*, **2016**, 45, 2823-2828.
33. S. W. Reilly, G. Akurathi, H. K. Box, H. U. Valle, T. K. Hollis, C. E. Webster. " $\beta$ -Boration of  $\alpha,\beta$ -unsaturated carbonyl compounds in ethanol and methanol catalyzed by CCC-NHC pincer Rh complexes" *J Organometallic Chem*, **2016**, 802, 32-38.
34. N. J. DeYonker, C. E. Webster. "The trans-cis Isomerization of  $Ni(\eta^2\text{-TEMPO})_2$ : Interconnections and Conformational Complexity" *Inorg Chim Acta*, **2015**, 436, 220-229.
35. G. E. Tyson, K. Tokmic, C. S. Oian, D. Rabinovich, H. U. Valle, T. K. Hollis, J. T. Kelly, K. A. Cuellar, L. E. McNamara, N. I. Hammer, M. Zhang, C. E. Webster, A. G. Oliver. "Synthesis, characterization, photophysical properties, and catalytic activity of an SCS bis(N-heterocyclic thione) (SCS-NHT) Pd pincer complex" *Dalton Trans*, **2015**, 44, 14475-14482.
36. N. J. DeYonker, C. E. Webster. "A Theoretical Study of Phosphoryl Transfers of Tyrosyl DNA-phosphodiesterase (Tdp1) and the Possibility of a 'Dead-End' Phosphohistidine Intermediate" *Biochemistry*, **2015**, 54, 4236-4247.
37. R. G. Letterman, C. B. Duke, III, T. T. To, T. J. Burkey, C. E. Webster. "Degenerate Pathways for Metallacycle Ring Inversions: A Common Phenomenon Consistent with the Principle of Microscopic Reversibility" *Organometallics*, **2014**, 33, 5928-5931.
38. M. Vennampalli, G. Liang, L. Katta, C. E. Webster, X. Zhao. "Electronic Effects on a Mononuclear Co Complex with a Pentadentate Ligand for Catalytic  $H_2$  Evolution" *Inorg Chem*, **2014**, 53, 10094-10100.
39. J. Gladysz, R. Bedford, M. Fujita, F. Gabbai, K. Goldberg, P. Holland, J. Kiplinger, M. Krische, J. Louie, C. Lu, J. Norton, M. Petrukhina, T. Ren, S. Stahl, D. Tilley, C. E. Webster, C. White, G. Whiteker. 2013 *Organometallics Roundtable*. *Organometallics*, **2014**, 33, 1505-1527.
40. T. R. Helgert, T. K. Hollis, A. G. Oliver, H. U. Valle, Y. Wu, C. E. Webster. "Synthesis, Characterization, and X-Ray Molecular Structure of Tantalum CCC-N-Heterocyclic Carbene (CCC-NHC) Pincer Complexes with Imidazole- and Triazole-Based Ligands" *Organometallics*, **2014**, 33, 952-958.
41. C. B. Duke, R. G. Letterman, J. O. Johnson, J. Barr, S. Hu, C. R. Ross, C. E. Webster, T. J. Burkey. "The Photochemistry of Arene Chromium Tricarbonyl Complexes with Tethered Pyridinyl and Propenyl Groups: Investigations of Chelate Formation, Structure, and Linkage Isomerization" *Organometallics*, **2014**, 33, 485-491.
42. M. Vennampalli, G. Liang, C. E. Webster, X. Zhao. "Water Oxidation by Mononuclear Ruthenium Complex with a Pentadentate Isoquinoline-Bipyridyl Ligand" *Eur J Inorg Chem*, **2014**, 715-721.
43. K. N. Leigh, C. E. Webster. "Theoretical Studies of Cyclic Adenosine Monophosphate dependent protein kinase: Native Enzyme and Ground-State and Transition-State Analogues" *Dalton Trans*, **2014**, 43, 3039-43. (DOI:10.1039/C3DT52358F)
44. D. Isrow, N. J. DeYonker, A. Koppaka, P. Pellechia, C. E. Webster, B. Captain. "Metal - Ligand Synergistic Effects in the Complex  $Ni(\eta^2\text{-TEMPO})_2$ . Synthesis, Structures, and Reactivity" *Inorg Chem*, **2013**, 52, 13882-13893.
45. M. Johnson, J. Thuman, R. G. Letterman, C. J. Stromberg, C. E. Webster, E. J. Heilweil. "Time-Resolved Infrared Studies of a Trimethylphosphine Model Derivative of [FeFe]-Hydrogenase" *J Phys Chem B*, **2013**, 117, 15792-15803. (DOI:10.1021/jp4067873)
46. N. J. DeYonker, C. E. Webster. "Phosphoryl Transfers of the Phospholipase D Superfamily: A Quantum Mechanical Theoretical Study" *J Am Chem Soc*, **2013**, 135, 13764-13774.
47. A. J. Huckaba, B. Cao, T. K. Hollis, H. U. Valle, J. T. Kelly, N. I. Hammer, A. G. Oliver, C. E. Webster. "Platinum CCC-NHC benzimidazolyl pincer complexes: synthesis, characterization, photostability, and theoretical investigation of a blue-green emitter" *Dalton Trans*, **2013**, 42, 8820-8826.
48. **Feature Article:** J. L. Bingaman, C. L. Kohnhorst, G. A. Van Meter, B. A. McElroy, E. A. Rakowski, B. C. Caplins, T. A. Gutowski, C. J. Stromberg, C. E. Webster, E. J. Heilweil. "Time-Resolved Vibrational Spectroscopy of [FeFe]-Hydrogenase Model Compounds" *J Phys Chem A*, **2012**, 116, 7261-7271.
49. W. M. Singh, T. Baine, S. Kudo, S. Tian, X. A. N. Ma, H. Zhou, N. J. DeYonker, T. C. Pham, J. C. Bollinger, D. L. Baker, B. Yan, C. E. Webster, X. Zhao. "Electrocatalytic and Photocatalytic Hydrogen Production in Aqueous Solution by a Molecular Cobalt Complex" *Angew Chem Int Ed*, **2012**, 51, 5941-5944.

50. J. L. Smeltz, C. E. Webster, E. Ison. "Computational Investigation of the Mechanism for the Activation of CO by Oxorhenium Complexes" *Organometallics*, **2012**, 31, 4055-4062.
51. J. L. Griffin, M. W. Bowler, N. J. Baxter, K. N. Leigh, H. R. W. Dannatt, A. M. Hounslow, G. M. Blackburn, C. E. Webster, M. J. Cliff, J. P. Waltho. "Near attack conformers dominate  $\beta$ -phosphoglucomutase complexes where geometry and charge distribution reflect those of substrate" *Proc Nat Acad Sci USA*, **2012**, 109, 6910-6915.
52. X. Zhang, A. M. Wright, N. J. DeYonker, T. K. Hollis, N. I. Hammer, C. E. Webster, E. J. Valente. "Synthesis, air stability, photobleaching, and DFT modeling of blue light emitting platinum CCC-N-heterocyclic carbene pincer complexes" *Organometallics* **2012**, 31, 1664-1672.
53. E. J. Heilweil, J. O. Johnson, K. L. Mosley, P. P. Lubet, C. E. Webster, T. J. Burkey. "Engineering Femtosecond Organometallic Chemistry: Photochemistry and Dynamics of Ultrafast Chelation of Cyclopentadienylmanganese Tricarbonyl Derivatives with Pendant Benzenecarbonyl and Pyridinecarbonyl Groups" *Organometallics* **2011**, 30, 5611-5619.
54. B. Radaram, J. A. Ivie, W. M. Singh, R. M. Grudzien, J. H. Reibenspies, C. E. Webster, X. Zhao. "Water Oxidation by Mononuclear Ruthenium Complexes with TPA-Based Ligands" *Inorg Chem*, **2011**, 50, 10564-10571.
55. S. M. Gittermann, R. G. Letterman, T. Jiao, G.-L. Leu, N. J. DeYonker, C. E. Webster, T. J. Burkey. "Bond Energies, Reaction Volumes, and Kinetics for  $\sigma$ - and  $\pi$ -Complexes of  $\text{Mo}(\text{CO})_5\text{L}$ " *J Phys Chem A*, **2011**, 115, 9004-9013.
56. B. H. G. Swennenhuis, R. Poland, N. J. DeYonker, C. E. Webster, D. J. Darensbourg, A. A. Bengali. "Ligand Displacement from  $\text{TpMn}(\text{CO})_2\text{L}$  Complexes: A Large Rate Enhancement in Comparison to the  $\text{CpMn}(\text{CO})_2\text{L}$  Analogues" *Organometallics*, **2011**, 30, 3054-3063.
57. K. R. Sawyer, J. F. Cahoon, J. E. Shanoski, E. A. Glascoe, M. F. Kling, J. P. Schlegel, M. C. Zoerb, M. Hapke, J. F. Hartwig, C. E. Webster, C. B. Harris. "Time-resolved IR studies on the mechanism for the functionalization of primary C-H bonds by Photoactivated  $\text{Cp}^*\text{W}(\text{CO})_3(\text{Bpin})$ " *J Am Chem Soc*, **2010**, 132, 1848-1859.
58. **Centennial Feature Article:** T. T. To, E. J. Heilweil, C. B. Duke, K. R. Ruddick, C. E. Webster, T. J. Burkey. "Development of Ultrafast Photochromic Organometallics and Photoinduced Linkage Isomerization of Arene Chromium Carbonyl Derivatives" *J Phys Chem A*, **2009**, 113, 2666-2676.
59. R. D. Adams, E. M. Boswell, B. Captain, S. Miao, C. Beddie, C. E. Webster, M. B. Hall, N. Dalal, N. Kaur, D. Zipse. "Disulfido iron-manganese carbonyl cluster complexes: Synthesis, structure, bonding and properties of the radical  $\text{CpFeMn}_2(\text{CO})_7(\mu^3\text{-S}_2)_2$ " *J Organometallic Chem* **2008**, 693, 2732-2738.
60. L. M. Pérez, C. E. Webster, A. A. Low, M. B. Hall. "Theoretical study of the biologically important dioxo diiron diamond core structures" *Theor Chem Acc* **2008**, 120, 467-478.
61. A. J. Blake, M. W. George, M. B. Hall, J. McMaster, P. Portius, X. Z. Sun, M. Towrie, C. E. Webster, C. Wilson, S. D. Zaric. "Probing the mechanism of carbon-hydrogen bond activation by photochemically generated hydridotris(pyrazolyl)borato carbonyl rhodium complexes: New experimental and theoretical investigations" *Organometallics* **2008**, 27, 189-201.
62. T. T. To, C. B. Duke, C. S. Junker, C. M. O'Brien, C. R. Ross, C. E. Barnes, C. E. Webster, T. J. Burkey. "Linkage isomerization as a mechanism for photochromic materials: Cyclopentadienylmanganese tricarbonyl derivatives with chelatable functional groups" *Organometallics* **2008**, 27, 289-296.
63. B. A. Vastine, C. E. Webster, M. B. Hall. "Carbon-hydrogen bond activation in hydridotris(pyrazolyl)borate Platinum(IV) complexes: Comparison of density functionals, basis sets, and bonding patterns" *J Chem Theory Comput* **2007**, 3, 2268-2281.
64. C. E. Webster. "Computational insights into degenerate ethylene exchange with a Grubbs-type catalyst" *J Am Chem Soc* **2007**, 129, 7490-7491.
65. C. E. Webster, M. B. Hall. "Forty Years of Fenske-Hall Molecular Orbital Theory" in *Theory and Applications of Computational Chemistry: The First 40 Years, A Volume of Technical and Historical Perspectives*, Editors: Clifford E. Dykstra, Gernot Frenking, Kwang S. Kim, and Gustavo Scuseria, Elsevier: New York, 2005, pp 1143-1165.
66. R. D. Adams, B. Captain, M. B. Hall, J. L. Smith, C. E. Webster. "High nuclearity iridium-platinum clusters: Synthesis, structures, bonding, and reactivity" *J Am Chem Soc* **2005**, 127, 1007-1014.
67. C. Beddie, C. E. Webster, M. B. Hall. "Urea decomposition facilitated by a urease model complex: a theoretical investigation" *Dalton Trans* **2005**, 3542-3551.
68. J. F. Hartwig, K. S. Cook, M. Hapke, C. D. Incarvito, Y. B. Fan, C. E. Webster, M. B. Hall. "Rhodium boryl complexes in the catalytic, terminal functionalization of alkanes" *J Am Chem Soc* **2005**, 127, 2538-2552.
69. C. E. Webster, C. L. Gross, D. M. Young, G. S. Girolami, A. J. Schultz, M. B. Hall, J. Eckert. "Electronic and steric effects on molecular dihydrogen activation in  $[\text{Cp}^*\text{OsH}_4(\text{L})]^+$  ( $\text{L} = \text{PPh}_3, \text{AsPh}_3, \text{and PCy}_3$ )" *J Am Chem Soc* **2005**, 127, 15091-15101.
70. R. D. Adams, B. Captain, W. Fu, M. B. Hall, J. Manson, M. D. Smith, C. E. Webster. "Bimetallic cluster complexes: The synthesis, structures, and bonding of ruthenium carbonyl cluster complexes containing palladium and platinum with the bulky tri-tert-butyl-phosphine ligand" *J Am Chem Soc* **2004**, 126, 5253-5267.
71. R. D. Adams, B. Captain, W. Fu, M. B. Hall, M. D. Smith, C. E. Webster. "Dinuclear ruthenium and iron complexes containing palladium and platinum with tri-tert-butylphosphine ligands: Synthesis, structures, and bonding" *Inorg Chem* **2004**, 43, 3921-3929.
72. R. D. Adams, B. Captain, J. L. Smith, M. B. Hall, C. L. Beddie, C. E. Webster. "Superloading of tin ligands into rhodium and iridium carbonyl cluster complexes" *Inorg Chem* **2004**, 43, 7576-7578.
73. R. D. Adams, S. Miao, M. D. Smith, H. Farach, C. E. Webster, J. Manson, M. B. Hall. "Nickel-manganese sulfido carbonyl cluster complexes. Synthesis, structure, and properties of the unusual paramagnetic complexes  $\text{Cp}_2\text{Ni}_2\text{Mn}(\text{CO})_3(\text{m}^3\text{-E})_2$ ,  $\text{E} = \text{S}, \text{Se}$ " *Inorg Chem* **2004**, 43, 2515-2525.
74. K. S. Cook, C. D. Incarvito, C. E. Webster, Y. B. Fan, M. B. Hall, J. F. Hartwig. "Rhodium silyl boryl hydride complexes: Comparison of bonding and the rates of elimination of borane, silane, and dihydrogen" **2004**, 43, 5474-5477.

75. H. D. Wang, C. E. Webster, L. M. Pérez, M. B. Hall, F. P. Gabbaï. "Reaction of the 1,8-bis(diphenylmethyl) naphthalenediyl dication with fluoride: Formation of a cation containing a C-F→C bridge" *J Am Chem Soc* **2004**, 126, 8189-8196.
76. C. E. Webster. "High-energy intermediate or stable transition state analogue: Theoretical perspective of the active site and mechanism of  $\beta$ -phosphoglucomutase" *J Am Chem Soc* **2004**, 126, 6840-6841.
77. C. E. Webster, M. Y. Darenbourg, P. A. Lindahl, M. B. Hall. "Structures and energetics of models for the active site of acetyl-coenzyme a synthase: Role of distal and proximal metals in catalysis" *J Am Chem Soc* **2004**, 126, 3410-3411.
78. G. Zampella, J. Y. Kravitz, C. E. Webster, P. Fantucci, M. B. Hall, H. A. Carlson, V. L. Pecoraro, L. De Gioia. "Quantum mechanical models of the resting state of the vanadium-dependent haloperoxidase" *Inorg Chem* **2004**, 43, 4127-4136.
79. K. A. Peterson, Y. M. Li, J. S. Francisco, P. Zou, C. E. Webster, L. M. Pérez, M. B. Hall, S. W. North. "The role of triplet states in the long wavelength absorption region of bromine nitrate" *J Chem Phys* **2003**, 119, 7864-7870.
80. C. E. Webster, Y. B. Fan, M. B. Hall, D. Kunz, J. F. Hartwig. "Experimental and computational evidence for a boron-assisted,  $\pi$ -bond metathesis pathway for alkane borylation" *J Am Chem Soc* **2003**, 125, 858-859.
81. C. E. Webster, M. B. Hall. "De Novo design in organometallic chemistry: stabilizing iridium(V)." *Coord Chem Rev* **2003**, 238, 315-331.
82. J. Eckert, C. E. Webster, M. B. Hall, A. Albinati, L. M. Venanzi. "The vibrational spectrum of Tp(3,5-Me)RhH<sub>2</sub>(H<sub>2</sub>): a computational and inelastic neutron scattering study" *Inorg Chim Acta* **2002**, 330, 240-249.
83. C. E. Webster, M. B. Hall. "Factors affecting the structure of substituted tris(pyrazolyl)borate rhodium dicarbonyl complexes" *Inorg Chim Acta* **2002**, 330, 268-282; **2002**, 336, 168-168.
84. C. E. Webster, M. B. Hall. "Theoretical studies of inorganic and organometallic reaction mechanisms. 20. Carbon-hydrogen and carbon-carbon bond activation of cyclopropane by cationic iridium(III) and neutral rhodium(I) and iridium(I) complexes" *Organometallics* **2001**, 20, 5606-5613.
85. C. E. Webster, M. B. Hall. "The theoretical transition state structure of a model complex bears a striking resemblance to the active site structure of DMSO reductase" *J Am Chem Soc* **2001**, 123, 5820-5821.
86. C. E. Webster, D. A. Singleton, M. J. Szymanski, M. B. Hall, C. Y. Zhao, G. C. Jia, Z. Y. Lin. "Minimum energy structure of hydridotris(pyrazolyl)borato iridium(V) tetrahydride is not a C<sub>3v</sub> capped octahedron" *J Am Chem Soc* **2001**, 123, 9822-9829.
87. C. R. Bowers, V. Storhaug, C. E. Webster, J. Bharatam, A. Cottone, R. Gianna, K. Betsey, B. J. Gaffney. "Exploring surfaces and cavities in lipoxxygenase and other proteins by hyperpolarized xenon-129 NMR" *J Am Chem Soc* **1999**, 121, 9370-9377.
88. S. Joerg, C. E. Webster, R. S. Drago, J. Sales. "Extension of the electrostatic-covalent model to 2:1 adducts" *Polyhedron* **1999**, 18, 1097-1106.
89. C. E. Webster, A. Cottone, R. S. Drago. "Multiple equilibrium analysis description of adsorption on Na-mordenite and H-mordenite" *J Am Chem Soc* **1999**, 121, 12127-12139.
90. C. E. Webster, R. S. Drago. "The multiple equilibrium analysis quantitative prediction of single and multi-component adsorption isotherms on carbonaceous and zeolitic solids" *Microporous Mesoporous Mater* **1999**, 33, 291-306.
91. C. E. Webster, R. S. Drago, M. C. Zerner. "A method for characterizing effective pore sizes of catalysts" *J Phys Chem B* **1999**, 103, 1242-1249.
92. C. E. Webster, J. P. Osegovic, B. J. Scott, S. C. Dias. "A thermodynamic analysis of the Cal-Ad method with respect to gas-solid calorimetry" *Microporous Mesoporous Mater* **1999**, 31, 205-209.
93. R. S. Drago, C. E. Webster, J. M. McGilvray. "A multiple-process equilibrium analysis of silica gel and HZSM-5" *J Am Chem Soc* **1998**, 120, 538-547.
94. C. E. Webster, R. S. Drago, M. C. Zerner. "Molecular dimensions for adsorptives" *J Am Chem Soc* **1998**, 120, 5509-5516.

## PATENTS

- T. K. Hollis, C. E. Webster, J. H. Delcamp, U.S. Pat. Appl. Publ. (2019), US 20190016741 A1 20190117. "Symmetrical CCC-NHC pincer metal complexes and symmetrical bimetallic complexes: bio-activity, and applications to organic transformations and energy-related catalytic methods"
- T. K. Hollis, C. E. Webster, PCT Int. Appl. (2018), WO 2018175659 A1 20180927. "Unsymmetrical salts, CCC-NHC pincer metal complexes, and methods of making the same"
- X. Zhao, C.E. Webster, U.S. Pat. Appl. Publ. (2015), US 20150021197 A1 20150122. "Novel metal complex catalysts and uses thereof including hydrogen production"
- X. Zhao, C. E. Webster, U.S. Pat. Appl. Publ. (2013), US 20130277229 A1 20131024. "Novel metal complex catalysts for hydrogen production"

## SOFTWARE

- JIMP 2, Manson, J.; Webster, C. E.; Pérez, L. M.; Hall, M. B. <http://www.chem.tamu.edu/jimp2/index.html>. Hall, M. B.; Fenske, R. F. *Inorg. Chem.* **1972**, 11, 768-779. Bursten, B. E.; Jensen, J. R.; Fenske, R. F. *J. Chem. Phys.* **1978**, 68, 3320.
- JIMP - The Interactive Molecule Program: Manson, J.; Webster, C. E.; Hall, M. B. <http://www.chem.tamu.edu/jimp>.

31 INVITED PRESENTATIONS

OVER 190 CONTRIBUTED PRESENTATIONS

OVER 20 OUTREACH ACTIVITIES WITH GREATER THAN 6000 PARTICIPANTS

MENTORING

- 1 research scientist
- 5 post-doctoral associates
- 24 graduate students
- 23 undergraduate students
- 5 high school students

**Service @ Department-Level:**

Current:

- Tenure-track Search Committee Chair
- Member of Space and Planning Committee
- Member of Undergraduate Affairs Committee
- Member of Graduate Affairs Committee
- Tenure and Promotion Committee

Previous:

- Graduate Coordinator (Three Years)
- Member of Graduate Studies Committee
- Tenure and Promotion Committee
- Faculty Mentor
- Technology Access Fee Software Liaison (Five Years)
- Departmental IT and Website Administrator (Five Years)
- Recruiting Chair on the Graduate Studies Committee (Four Years)
- Seminar Chair (One Year)
- Seminar Co-Chair (One Year)
- Organize and Co-Organize Undergraduate Research Conference (Two Years)
- Staff Scientist Search Committee
- Faculty Third Year Review Committee
- Faculty Search Committees

**Service @ College-Level:**

Previous:

- Graduate Council for the College of Arts and Sciences (Three Years)
- Selection Committee for the College of Arts and Sciences Travel Enrichment Funds (Five Semesters Over Three Years)
- Selection Committee for the College of Arts and Sciences Graduate Student Awards (One Semester)

**Service @ University-Level:**

Current:

- IT Security Assessment Planning Group
- International Institute Advisory Board Member

Previous:

- Director of the Computational Research On Materials Institute At The University Of Memphis (CROMIUM) (Three Years)
- Information Technology Research Advisory Committee (ITRAC) (Five Years)
- ITRAC High Performance Computing Subcommittee (Five Years)
- Facilities Director for CROMIUM (Five Years)
- ITRAC High Performance Computing Subcommittee (Chair, One Year)
- ITRAC High Performance Computing Request for Proposals Evaluation Committee (twice, each time the RFP was offered while I was at U of M)
- Teaching and Learning Advisory Committee (TLAC) (Two Years)
- Faculty Advisory Committee for Research (Two Years)

## INVITED PRESENTATIONS

- C. E. Webster "Interpreting Time-Resolved Spectra and Excited State Reactivity with DFT and TD-DFT" Catalysis/Mid-Career Quantum Chemistry Meeting, Texas A&M University, Doha, Qatar, March 10-11, 2019.
- C. E. Webster "Investigations in Computational Inorganic and Organometallic Photochemistry and Photophysics" Tulane University, New Orleans, LA, February 26, 2018.
- C. E. Webster, G. Liang, T. R. Helgert, J. A. Denny, G. M. Lang, T. K. Hollis. "Extreme  $\pi$ -loading and imido reactivity in CCC-NHC Ta bis(imido) pincer complexes" Silver Anniversary of N-Heterocyclic Carbenes Symposium, Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-600.
- C. E. Webster, G. Liang, T. R. Helgert, J. A. Denny, G. M. Lang, T. K. Hollis. "Computational study of extreme  $\pi$ -loading and imido reactivity in CCC-NHC Ta bis(imido) pincer" Invited lecture, Computational Chemistry Meeting, Environmental Laboratory, Engineer Research and Development Center, September 12, 2017, Vicksburg, MS.
- E. V. Dornshuld, C. E. Webster. "Computational Chemistry: A Primer" Feeding and Powering the World 2017: Building the Knowledge Base, June 19-20, 2017, The University of Mississippi, Oxford, MS.
- C. E. Webster. "Challenges in Computational Transition Metal Chemistry" Invited lecture, Feeding and Powering the World 2016: Building the Network, July 25-26, 2016, The University of Mississippi, Oxford, MS.
- C. E. Webster. "Theoretical studies of phosphoryl transfer enzymes" Invited lecture, 8th Mississippi Regional Biophysical Consortium, June 3-4, 2015, The University of Mississippi, Oxford, MS.
- C. E. Webster. "Forays into Computational Chemistry" Invited lecture, Alumni Summer Symposium, August 7 2014, University of West Florida, Pensacola, FL.
- C. E. Webster. "Computational design of organometallic photochromic systems" Invited lecture, Breaking and Making Bonds with Light, June 30 - July 4 2014, Telluride Science Research Center, Telluride, CO.
- K. N. Leigh, W. D. Clark, T. K. Hollis, C. E. Webster. "Mechanistic studies of intramolecular hydroamination of alkylamines by a zirconium(IV) CCC-NHC pincer complex" Southwest Regional Meeting (SWRM) 2013, Waco, TX, November 16-19, 2013.
- W. D. Clark, J. Cho, H. U. Valle, T. R. Helgert, T. K. Hollis, E. J. Valente, K. N. Leigh, C. E. Webster. "Mechanistic investigations in the hydroamination/cyclization of unactivated amino-alkenes with a CCC-NHC Zr pincer complex" Southwest Regional Meeting (SWRM) 2013, Waco, TX, November 16-19, 2013 (presented by T. K. Hollis).
- C. E. Webster, K. N. Leigh, R. G. Letterman, N. J. DeYonker. "Phosphoryl transfer enzymes: theoretical studies of native enzymes and ground-state and transition-state analogues" Southwest Regional Meeting (SWRM) 2013, Waco, TX, November 16-19, 2013.
- C. E. Webster, N. J. DeYonker, D. Isrow, A. Koppaka, B. Captain. "Metal - ligand synergistic effects in Ni( $\eta^2$ -TEMPO)<sub>2</sub>, structures and reactivity" 89th Annual Florida Annual Meeting and Exposition, FAME 2013, Innisbrook, FL, May 9-11, 2013.
- C. E. Webster. "Designing and engineering organometallic photochromic systems with chelating, bifunctional tethered side-chains" Invited lecture, October 24, 2012, seminar presented at Texas A&M University, College Station, TX.
- C. E. Webster. "Computational design of organometallic photochromic systems" Invited lecture, Breaking and Making Bonds with Light, July 2-6 2012, Telluride Science Research Center, Telluride, CO.
- C. E. Webster. "Computational design of organometallic photochromic systems" Invited lecture, February 10, 2012, seminar presented at Mississippi State University, Starkville, MS.
- C. E. Webster, K. R. Ruddick, K. L. Mosley, J. O. Johnson, P. P. Lubet, E.J. Heilweil, T. J. Burkey. "Computational design of organometallic photochromic systems with chelating, bifunctional tethered side-chains." Abstracts of Papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010, COMP-331.
- C. E. Webster. "Applications of Density Functional Theory: Research Snapshots of  $\beta$ -phosphoglucomutase and DMSO reductase" Invited lecture, November 21, 2008, seminar presented at the University of Southern Mississippi, Hattiesburg, MS.
- C. E. Webster. "Forays into Computational Chemistry" Invited lecture, seminar presented at Bartlesville Technology Center, ConocoPhillips Inc., Bartlesville, OK, April 15, 2008.
- C. E. Webster. "Separating electronic, steric, and packing interactions utilizing Density Functional Theory (or Not!)" Invited lecture, seminar presented at the University of Alabama, Birmingham, Birmingham, AL, February 21, 2008.
- C. E. Webster. "Theoretical study of the active site and mechanism of  $\beta$ -phosphoglucomutase" Invited lecture, June 17-22, 2007, Biocatalysis 2007, Moscow to, St. Petersburg, Russia.
- C. E. Webster. "Theoretical study of the active site and mechanism of  $\beta$ -phosphoglucomutase" 17th International Conference on Phosphorus Chemistry April 15-21, 2007, Xiamen University, Xiamen, P.R. China.
- C. E. Webster. "Theoretical study of the active site and mechanism of  $\beta$ -phosphoglucomutase" Invited lecture, April 22-23, 2007, Zhengzhou University, Dept. of Chemistry, Zhengzhou, P.R. China.
- C. E. Webster. "Theoretical study of the active site and mechanism of  $\beta$ -phosphoglucomutase" Invited lecture April 24-25, 2007, Tsinghua University, Dept. of Chemistry, Beijing, P.R. China.
- C. E. Webster. "Continuing the renaissance in inorganic chemistry: Drago's Physical Methods in Inorganic Chemistry" Abstracts of Papers, 233rd ACS National Meeting, Chicago, IL, United States, March 25-29, 2007 (2007), HIST-010.
- C. E. Webster. "Separating electronic, steric, and packing interactions utilizing Density Functional Theory (or Not!)" Invited lecture, September 28, 2006, seminar presented at the University of Mississippi, Oxford, MS.
- C. E. Webster. "Applications of Density Functional Theory: Research Snapshots" Invited lecture, March 2, 2006, seminar presented at the Middle Tennessee State University, Murfreesboro, TN.



- C. E. Webster. "Theoretical Investigations into the Active Site Structure and Mechanism of Dimethylsulfoxide Reductase" Recruiting seminar, March 1, 2006, presented at the Middle Tennessee State University, Murfreesboro, TN.
- C. E. Webster, M. B. Hall. "Theoretical Studies of the Reaction Mechanism of Dimethylsulfoxide Reductase with Inorganic Model Complexes" Invited lecture, September 17, 2003, seminar presented at the Biophysical Night Out, College Station, Texas.
- C. E. Webster. "Modeling Adsorption: Investigating Adsorbate and Adsorbent Properties" Invited lecture, January 29, 1999, seminar presented at the University of West Florida, Pensacola, FL.

## CONTRIBUTED PRESENTATIONS

- C. E. Webster, G. Liang, T. R. Helgert, J. A. Denny, G. M. Lang, T. K. Hollis. "Computational study of extreme  $\pi$ -loading and imido reactivity in CCC-NHC Ta bis(imido) pincer complexes" Abstracts of Papers, 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017 (2017), INOR-599.
- C. E. Webster, K. N. Leigh, R. G. Letterman, N. J. DeYonker. "Phosphoryl transfer enzymes: Theoretical studies of native enzymes and ground-state and transition-state analogs" Abstracts of Papers, 247th ACS National Meeting & Exposition, Dallas, TX, United States, March 16-20, 2014 (2014), INOR-41.
- C. E. Webster, N. J. DeYonker. "The many phosphoryl transfers of Phospholipase D superfamily: A quantum mechanical theoretical study" 89th Annual Florida Annual Meeting and Exposition, FAME 2013, Innisbrook, FL, May 9-11, 2013.
- C. E. Webster, R. G. Letterman, J. W. Barr, J. O. Johnson, T. M. McFadden, C. B. Duke, T. To, T. J. Burkey. "Designing and engineering organometallic photochromic systems with chelating, bifunctional tethered side-chains" Abstracts of Papers, 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013 (2013), INOR-1086.
- C. E. Webster. "The many phosphoryl transfers of Phospholipase D superfamily: A quantum mechanical theoretical study" SouthWest Theoretical Chemistry Conference, College Station, TX, October 27-28, 2012.
- R. G. Letterman, C. B. Duke, T. T. To, T. J. Burkey, C. E. Webster. "How do inequivalent atoms in an organometallic complex become equivalent on the NMR timescale?" Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012, INOR-354.
- K. N. Leigh, T. K. Hollis, C. E. Webster. "Computational study of catalytic intramolecular hydroamination by a CCC-NHC Rh pincer complex" Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012, INOR-232.
- R. G. Letterman, N. J. DeYonker, T. J. Burkey, C. E. Webster. "Should density functional theory be used to guide the design of chromium-containing photochromic materials?" Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012, INOR-224.
- K. N. Leigh, J. P. Waltho, G. M. Blackburn, M. W. Bowler, C. E. Webster. "Utilization of computed  $^{19}\text{F}$  NMR to identify active site intermediate and transition-state analogs in  $\beta$ -PGM" Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012, INOR-55.
- C. E. Webster, N. J. DeYonker. "The many phosphoryl transfers of Phospholipase D: A quantum mechanical theoretical study" Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012, INOR-54.
- K. N. Leigh, C. E. Webster. "Computational study of catalytic intramolecular hydroamination by a CCC-NHC Rh pincer complex" SETCA 2012, May 17-19, 2012, Athens, GA.
- R. G. Letterman, N. J. DeYonker, T. J. Burkey, C. E. Webster. "Should density functional theory be used to guide the design of chromium-containing photochromic materials?" SETCA 2012, May 17-19, 2012, Athens, GA.
- M. Yang, N. J. DeYonker, X. Zhao, C. E. Webster. "Computational Reduction Potentials of Ferrocene and Cobaltocene Derivatives" SETCA 2012, May 17-19, 2012, Athens, GA.
- K. Leigh, C. E. Webster. "Theoretical study of the active site and mechanism of  $\beta$ -phosphoglucomutase and phosphoserine phosphatase" Abstracts of Papers, 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010, INOR-37.
- C. E. Webster. "Computational insights into degenerate ethylene exchange with a Grubbs type catalyst" Midsouth Inorganic Chemists Association held at Harding University, Searcy, AR, October 13, 2007.
- C. E. Webster. "Computational insights into degenerate ethylene exchange with a Grubbs type catalyst" Abstracts of Papers, 234th ACS National Meeting, Boston, MA, United States, August 19-23, 2007 (2007), INOR-018.
- C. E. Webster. "Theoretical study of the active site and mechanism of  $\beta$ -phosphoglucomutase" Abstracts of Papers, 233rd ACS National Meeting, Chicago, IL, United States, March 25-29, 2007 (2007), INOR-223.
- C. E. Webster, M. Y. Darenbourg, P. A. Lindahl, M. B. Hall. "Structures and Energetics of Models for the Active Site of Acetyl-Coenzyme A Synthase: Role of Distal and Proximal Metals in Catalysis." Abstracts, 60th Southwest Regional Meeting of the American Chemical Society, Fort Worth, TX, United States, September 29-October 4, 2004, SEPT04-110.
- M. B. Hall, C. E. Webster. "Separating Electronic, Steric, and Packing Interactions in Crystallographic Structures by Density Functional Theory." Abstracts, 60th Southwest Regional Meeting of the American Chemical Society, Fort Worth, TX, United States, September 29-October 4, 2004, SEPT04-088.
- C. E. Webster, M. B. Hall. "Theoretical Studies of the Molybdenum Oxotransferase Enzymes"—Poster presented at Molybdenum & Tungsten Enzymes, Gordon Research Conference, Kimball Union Academy, Meriden, New Hampshire June 29-July 4, 2003.
- C. E. Webster, M. B. Hall. "Factors affecting the structure of substituted tris(pyrazolyl)borato rhodium dicarbonyl complexes." Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002, INOR-293, 223, A50.
- C. E. Webster, M. B. Hall. "Carbon-hydrogen and carbon-carbon bond activation of cyclopropane by a cationic iridium(III) complex, a theoretical study." Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002, INOR-357, 223, A60.
- C. E. Webster, M. B. Hall. "Theoretical transition state structure of a model complex bears a striking resemblance to the active site structure of DMSO reductase." Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002, INOR-404, 223, A67.
- C. E. Webster, M. B. Hall. "Elongated Dihydrogen?  $\text{ReH}_7(\text{p-tol})_3$  Revisited"—Seminar presented at the Computational Chemistry Users Meeting, Environmental Molecular Sciences Laboratory at the Pacific Northwest National Laboratory, Richland, Washington, June 18-19, 2001.

- C. E. Webster, M. B. Hall. "A theoretical study of carbon-hydrogen and carbon-carbon bond activation of cyclopropane by a cationic iridium(III) complex"—Poster presented at the 17th Southwest Theoretical Chemistry Conference (17th SWTCC), College Station, TX, November 2-4, 2000.
- C. E. Webster, M. B. Hall. "Computational Studies of Tris(pyrazolyl)borate Complexes of Iridium"—Poster presented at the Contemporary Inorganic Chemistry-II (CIC-II), College Station, TX, March 12-15, 2000.
- C. E. Webster, M. B. Hall. "Theoretical study of the reaction mechanism of dimethylsulfoxide reductase, a molybdenum-containing oxotransferase enzyme." Abstracts of Papers, 220th ACS National Meeting, Washington, DC, United States, August 20-24, 2000, INOR-416, 220, U515.
- C. E. Webster, R. S. Drago, M. C. Zerner. "The Multiple Equilibrium Analysis Description of Adsorption on HZSM-5"—Seminar presented at the Florida American Chemical Society Meeting and Exposition (FAME 99), Orlando, FL, May 8-9, 1999.
- C. E. Webster, J. P. Osegovic, C.R. Bowers. "Deuteron Quadrupole Spin Echo NMR of *d*<sub>5</sub>-Pyridine Chemisorbed on Zeolites"—Poster presented at the 40th Experimental Nuclear Magnetic Resonance Conference (ENC), Orlando, FL, February 28-March 5, 1999.
- C. E. Webster, R. S. Drago, M. C. Zerner. "A Method for Determining the Effective Catalytic Pore Size of HZSM-5"—Poster presented at the Florida American Chemical Society Meeting and Exposition (FAME 98), Orlando, FL, May 8-9, 1998.
- C. E. Webster, R. S. Drago, M. C. Zerner. "Modeling Adsorption: A Method for Characterizing the Effective Catalytic Pore Size of HZSM-5"—Poster presented at the Florida Catalysis Conference; Palm Coast, FL, April 27, 1998.

#### CONTRIBUTED PRESENTATIONS BY COLLABORATORS

- D. B. Burks, R. W. Lamb, S. Das, C. M. Boudreaux, C. E. Webster, E. T. Papish, "Mechanistic Studies of Ruthenium CNC-Pincer Complexes for Carbon Dioxide Reduction Catalysis" Feeding and Powering the World 2019: The Next Generation, July 15-16, 2019, The University of Mississippi, Oxford, MS.
- P. Wang, G. Liang, E. Towles, D. Li, C. Boyd, K. Hill, B. Shaver, W. Grubbs, C. E. Webster, and X. Zhao. "Molecular cobalt complexes with pentadentate ligands for electro- and photocatalytic hydrogen generation in aqueous solution" Abstracts of Papers, 258th ACS National Meeting & Exposition, San Diego, CA, United States, August 25-29, 2019 (2019), INOR-0602.
- S. Autry, M. Zhang, E. Dornshuld, T. K. Hollis, C. E. Webster, H. Hammer. "Probing the effects of environment on novel CCC-NHC-Pt(II) pincer complexes" Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019 (2019), YCC-0026.
- E. T. Papish, S. Das, C. M. Boudreaux, D. B. Burks, R. R. Rodrigues, C. E. Webster, J. H. Delcamp. "Pyridinol-based CNC Pincer catalysts for carbon dioxide reduction: The big impact of one small remote group" Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019 (2019), INOR-0536.
- E. Caldon, M. Zhang, T. K. Hollis, C. E. Webster, D. Wipf, D. W. Smith. "Corrosion inhibition of mild steel in acidic medium by simple triazole- and imidazole-based aromatic compounds" Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019 (2019), ANYL-0367.
- R. Adams, A. Griffith, G. Liang, C. E. Webster, R. H. Schmehl. "Identification of the intermediates and products formed during osmium hydride protonation in acetonitrile" Feeding and Powering the World 2018: Planning for the Future, July 16-17, 2018, The University of Mississippi, Oxford, MS.
- S. Autry, M. Zhang, J. Gayton, T. K. Hollis, C. E. Webster, J. Delcamp, N. I. Hammer. "Spectroscopic Characterization of Newly Developed Systems and Challenges to Overcome" Feeding and Powering the World 2018: Planning for the Future, July 16-17, 2018, The University of Mississippi, Oxford, MS.
- S. Davis, D. Burks, R. W. Lamb, X. Liu, R. R. Rodrigues, N. P. Liyanage, Y. Sun, C. E. Webster, E. T. Papish, J. H. Delcamp. "Nickel(II) Pincer Complexes Demonstrate that the Remote Substituent Controls Catalytic Carbon Dioxide Reduction" Feeding and Powering the World 2018: Planning for the Future, July 16-17, 2018, The University of Mississippi, Oxford, MS.
- G. Ragunathan, P. R. Fontenot, B. Shan, B. Wang, A. Obanda, A. F. Greene, J. T. Mague, L. A. Hunt, N. Hammer, P. Shinde, S. Pan, C. E. Webster, R. H. Schmehl, J. P. Donahue. "New Developments in Catalytic H<sub>2</sub> -Formation by Molybdenum Sulfide Clusters" Feeding and Powering the World 2018: Planning for the Future, July 16-17, 2018, The University of Mississippi, Oxford, MS.
- H. P. Shirley, A. J. Huckaba, R. W. Lamb, S. Guertin, S. Autry, H. Cheema, K. Talukdar, T. Jones, J. W. Jurss, A. Dass, N. I. Hammer, R. H. Schmehl, C. E. Webster, J. H. Delcamp. "A Novel Homogeneous Tungsten Catalyst for the Photocatalytic production of H<sub>2</sub>" Feeding and Powering the World 2018: Planning for the Future, July 16-17, 2018, The University of Mississippi, Oxford, MS.
- A. Huckaba, H. P. Shirley, R. W. Lamb, S. L. Guertin, S. Autry, H. A. Cheema, K. Talukdar, Jones, Tanya C.; J. W. Jurss, A. Dass, N. Hammer, R. H. Schmehl, C. E. Webster, J. H. Delcamp "Investigation into the mechanism of proton reduction catalysis by chromophore-catalyst [W(PyNHCPhCF<sub>3</sub>)(CO)<sub>4</sub>]" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-508.
- H. P. Shirley, A. Huckaba, R. W. Lamb, S. L. Guertin, S. Autry, H. A. Cheema, K. Talukdar, Jones, Tanya C.; J. W. Jurss, A. Antonysamy, N. Hammer, R. H. Schmehl, C. E. Webster, J. H. Delcamp "Photocatalytic H<sub>2</sub> production via a homogeneous tungsten catalyst" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-1268.
- E. T. Papish, D. B. Burks, S. Siek, A. J. Curto, G. Liang, S. Autry, J. Shankwitz, C. E. Webster, N. Hammer, G. Szulczewski. "Metal complexes of 6,6'-dihydroxybipyridine catalyze energy related transformations including water oxidation and carbon dioxide reduction" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-385.

- X. Zhao, P. Wang, G. Liang, M. Long, D. Reese, A. Bah, C. C. James, Y. Sun, L. Duan, C. E. Webster. "Electronic and steric effects on hydrogen production catalyzed by molecular Co complexes with pentadentate ligands in aqueous solution" Abstracts of Papers, 254th ACS National Meeting & Exposition, Washington, DC, USA, August 20-24, 2017 (2017), INOR-904.
- S. L. Guertin, A. J. Huckaba, H. Shirley, R. Lamb, S. Autry, H. Cheema, K. Talukdar, T. Jones, J. W. Jurss, A. Dass, N. I. Hammer, R. H. Schmehl, C. E. Webster, J. H. Delcamp. "Investigation into the Mechanism of Proton Reduction Catalysis by Chromophore-Catalyst [W(PyNHCPhCF<sub>3</sub>)(CO)<sub>4</sub>]" Feeding and Powering the World 2017: Building the Knowledge Base, June 19-20, 2017, The University of Mississippi, Oxford, MS.
- S. A. Autry, M. Zhang, V. Dixit, T. K. Hollis, C. E. Webster, N. I. Hammer. "Spectroscopic Characterization of the Physical and Photophysical Properties of Newly Developed Platinum Pincer Complexes" Feeding and Powering the World 2017: Building the Knowledge Base, June 19-20, 2017, The University of Mississippi, Oxford, MS.
- R. Adams, T. A. Grusenmeyer, G. Liang, C. E. Webster, R. H. Schmehl. "Dramatically Enhanced Hydride Protonation Rates following Photoinduced One Electron Reduction of Os(II) Hydride Complexes" Feeding and Powering the World 2017: Building the Knowledge Base, June 19-20, 2017, The University of Mississippi, Oxford, MS.
- S. A. Autry, M. Zhang, V. Dixit, T. K. Hollis, C. E. Webster, N. Hammer. "Spectroscopic characterization of the physical and photo-physical properties of newly developed platinum pincer complexes" Abstracts of Papers, 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017 (2017), PHYS-456.
- X. Zhao, Xuan; P. Ping; Y. Yue; L. Lian; M. Long, D. Reese, A. Bah, C. James, G. Liang, C. E. Webster. "Electro- and photolytic hydrogen production catalyzed by molecular Co complexes with pentadentate ligands in aqueous solution" Abstracts of Papers, 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017 (2017), INOR-1369.
- E. T. Papish, S. Siek, D. B. Burks, C. Boudreaux, D. L. Gerlach, G. Liang, D. B. Grotjahn, C. E. Webster. "Pyridinol based ligands for transition metal catalyzed reduction of CO<sub>2</sub> and related substrates: Elucidating the role of Lewis Acids" Abstracts of Papers, 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017 (2017), INOR-614.
- X. Zhao, S. Powers, P. Wang, R. Mittapalli, K. Knight, T. Rice, C. Lyons, K. Driskill, G. Liang, C. E. Webster. "Hydrogen production catalyzed by molecular Co complexes with pentadentate ligands" Abstracts of Papers, 252nd ACS National Meeting & Exposition, Philadelphia, PA, United States, August 21-25, 2016 (2016), INOR-53.
- H. P. Shirley, H. Cheema, T. Jones, A. J. Huckaba, A. Dass, C. E. Webster, J. H. Delcamp. "Photocatalytic H<sub>2</sub> Production Via Tungsten Catalyst" Feeding and Powering the World 2016: Building the Network, The University of Mississippi, Oxford, MS, July 25-26, 2016.
- X. Zhao, M. Yanney, M. Vennampalli, G. Liang, C. E. Webster. "Electro- and photolytic hydrogen production by mononuclear cobalt complexes with pentadentate ligands" Preprints - American Chemical Society, Division of Energy & Fuels (2015), 60(2), 299-300.
- X. Zhao, M. Yanney, M. Vennampalli, G. Liang, C. E. Webster. "Electro- and photolytic hydrogen production by mononuclear cobalt complexes with pentadentate ligands" Abstracts of Papers, 250th ACS National Meeting & Exposition, Boston, MA, United States, August 16-20, 2015 (2015), ENFL-182.
- X. Zhao, M. Vennampalli, G. Liang, L. Katta, C. E. Webster. "Electronic tuning of H<sub>2</sub> production catalyzed by Co complexes with pentadentate ligands" Abstracts of Papers, 249th ACS National Meeting & Exposition, Denver, CO, United States, March 22-26, 2015 (2015), INOR-873.
- W. D. Clark, T. K. Hollis, K. N. Leigh, C. E. Webster. "Mechanistic investigations in the hydroamination/cyclization of unactivated amino-alkenes with CCC-NHC Zr pincer complexes" Abstracts, 49th Midwest Regional Meeting of the American Chemical Society, Columbia, MO, United States, November 12-15 (2014), MWRM-451.
- T. K. Hollis, C. E. Webster, T. R. Helgert, H. K. Box, H. U. Valle, A. G. Oliver, W. D. Clark. "Next generation ligand architectures: CCC-NHC pincer Ta complexes; synthetic methods and applications" Abstracts, 49th Midwest Regional Meeting of the American Chemical Society, Columbia, MO, United States, November 12-15 (2014), MWRM-260.
- X. Zhao, M. Vennampalli, G. Liang, M. Zhang, C. E. Webster. "Electronic effect on catalytic H<sub>2</sub> production by Co complexes with pentadentate ligands" Abstracts of Papers, 248th ACS National Meeting & Exposition, San Francisco, CA, United States, August 10-14, 2014 (2014), INOR-1083.
- X. Zhao, M. Vennampalli, C. Que, T. Baine, M. Zhang, G. Liang, J. C. Bollinger, C. E. Webster. "Electro- and photocatalytic H<sub>2</sub> production by Co complexes with pentadentate ligands" Abstracts of Papers, 247th ACS National Meeting & Exposition, Dallas, TX, United States, March 16-20, 2014 (2014), INOR-837.
- J. O. Johnson, R. G. Letterman, E. J. Heilweil, C. E. Webster, T. J. Burkey. "Synthesis and characterization of (η<sup>5</sup>-Pentalenyl)Mn(CO)<sub>2</sub> complexes with tethered functional groups: Development of organometallic photochromes" Abstracts of Papers, 247th ACS National Meeting & Exposition, Dallas, TX, United States, March 16-20, 2014 (2014), INOR-286.
- M. Silkowski, N. J. DeYonker, C. E. Webster, X. Zhao, G. R. Shelton. "Synthesis and characterization of ligands for organometallic biomimetic catalysts" Abstracts of Papers, 247th ACS National Meeting & Exposition, Dallas, TX, United States, March 16-20, 2014 (2014), CHED-1133.
- L. T. Nguyen, N. J. DeYonker, C. E. Webster, X. Zhao, G. R. Shelton. "In silico de novo development and design of ligands for organometallic biomimetic catalysts" Abstracts of Papers, 247th ACS National Meeting & Exposition, Dallas, TX, United States, March 16-20, 2014 (2014), CHED-639.
- (Invited) W. D. Clark, J. Cho, H. U. Valle, T. R. Helgert, T. K. Hollis, E. J. Valente, K. N. Leigh, C. E. Webster. "Mechanistic investigations in the hydroamination/cyclization of unactivated amino-alkenes with a CCC-NHC Zr pincer complex" Abstracts, 69th Southwest Regional Meeting of the American Chemical Society, Waco, TX, United States, November 16-19 (2013), SWRM-568.

- G. E. Tyson, K. Tokmic, D. Rabinovich, H. U. Valle, T. K. Hollis, C. E. Webster, J. T. Kelly, N. I. Hammer. "Synthesis, characterization, and photophysical properties of a novel bis(N-heterocyclic thione) (NHT's) SCS-Pd pincer complex" Abstracts, 65th Southeast Regional Meeting of the American Chemical Society, Atlanta, GA, United States, November 13-16 (2013), SERM-757.
- T. R. Helgert, T. K. Hollis, A. G. Oliver, H. U. Valle, Y. Wu, C. E. Webster. "CCC-NHC Pincer Ta (V) Complexes: Synthesis, Ligand Exchange, NHC Rearrangement to a Mixed NHC-MIC (Mesoionic Carbene) Pincer, and Intramolecular Catalytic Oxidative Hydroamination of Alkenes" Abstracts, 65th Southeast Regional Meeting of the American Chemical Society, Atlanta, GA, United States, November 13-16 (2013), SERM-590.
- W. D. Clark, J. Cho, H. U. Valle, T. R. Helgert, T. K. Hollis, E. J. Valente, K. N. Leigh, C. E. Webster. "Mechanistic investigations in the hydroamination/cyclization of unactivated amino-alkenes with a CCC-NHC Zr pincer complex" Abstracts, 65th Southeast Regional Meeting of the American Chemical Society, Atlanta, GA, United States, November 13-16 (2013), SERM-158.
- M. Zhang, Min; C. Xie, G. Liang, J. C. Bollinger, C. E. Webster, X. Zhao. "Synthesis and characterization of metal complexes with pentadentate ligands for catalytic H<sub>2</sub> evolution" Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013 (2013), INOR-158.
- M. Vennampalli, G. Liang, J. C. Bollinger, C. E. Webster, X. Zhao. "Design of mononuclear metal complexes with polypyridyl ligands for catalytic H<sub>2</sub> production" Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013 (2013), INOR-159.
- B. Captain, A. Koppaka, D. Isrow, N. J. DeYonker, C. E. Webster. "Small molecule activation by the nitroxide containing complex Ni( $\eta^2$ -TEMPO)<sub>2</sub>" Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013 (2013), INOR-216.
- X. Zhao, M. Vennampalli, C. Que, T. Baine, M. Zhang, G. Liang, C. Xie, J. C. Bollinger, C. E. Webster. "Design of molecular metal complexes with polydentate ligands for H<sub>2</sub> production" Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013 (2013), INOR-484.
- C. Que, H. Duan, M. Yang, K. Abubakar, J. C. Bollinger, B. Yan, C. E. Webster, X. Zhao. "Mononuclear nickel polypyridine complex as robust electro- and photocatalyst for H<sub>2</sub> production" Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013 (2013), INOR-485.
- M. Vennampalli, C. Que, T. Baine, M. Zhang, J. C. Bollinger, C. E. Webster, X. Zhao. "Catalytic water splitting by metal complexes based on tris(2-pyridylmethyl)amine derivatives" Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013 (2013), ENFL-117.
- E. J. Heilweil, T. J. Burkey, J. O. Johnson, R. G. Letterman, C. E. Webster. "Design of organometallic photochromes: Utilizing linkage isomerization in the production of ultrafast devices" Abstracts of Papers, 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013 (2013), INOR-774.
- J. O. Johnson, K. L. Mosley, R. G. Letterman, P. P. Lubet, C. E. Webster, T. J. Burkey. "Synthesis and properties of organometallic photochromes based on ( $\eta^5$ -cyclopentadienyl)Mn(CO)<sub>3</sub> and ( $\eta^5$ -pentalenyl)Mn(CO)<sub>3</sub> complexes" Abstracts of Papers, 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013 (2013), INOR-731.
- X. Zhao, H. Duan, C. Que, M. Yang, K. Abubakar, D. L. Baker, B. Yan, C. E. Webster. "Hydrogen evolution catalyzed by molecular nickel complex with DPA-Bpy ligand" Abstracts of Papers, 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013 (2013), INOR-712.
- T. Baine, W. M. Singh, S. Kudo, S. Tian, H. Zhou, N. J. DeYonker, T. C. Pham, J. C. Bollinger, D. L. Baker, B. Yan, Y. Lu, C. E. Webster, X. Zhao. "Electrocatalytic and photocatalytic hydrogen production in aqueous solution by a molecular cobalt complex" Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012 (2012), INOR-521.
- X. Zhao, W. M. Singh, T. Baine, C. E. Webster, B. Yan, S. Tian, H. Zhou. "Hydrogen evolution catalyzed by molecular cobalt complexes in aqueous solution" Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012 (2012), INOR-18.
- T. Baine, W. M. Singh, S. Kudo, S. Tian, X. A. N. Ma, H. Zhou, N. J. DeYonker, T. C. Pham, J. C. Bollinger, D. L. Baker, B. Yan, C. E. Webster, X. Zhao. "Electrocatalytic and Photocatalytic Hydrogen Production in Aqueous Solution by a Molecular Cobalt Complex" The TN-SCORE Annual Conference, Vanderbilt Marriot, Nashville, June 15, 2012.
- T. J. Burkey, E. J. Heilweil, J. O. Johnson, K. L. Mosley, P. P. Lubet, C. E. Webster. "Preparation and photochemistry of cyclopentadienyl manganese tricarbonyl derivatives with pendant hydrazone and pyridine groups" Abstracts of Papers, 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-March 29, 2012 (2012), INOR-1001.
- T. J. Burkey, C. B. Duke, R. G. Letterman, C. R. Ross, C. E. Webster. "Synthetic, structural, photochemical, and thermochemical studies of arene chromium tricarbonyl complexes with tethered pyridine groups" Abstracts of Papers, 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-March 29, 2012 (2012), INOR-1000.
- C. Que, M. Singh, C. E. Webster, X. Zhao. "Water oxidation by metal complexes with tris(2-pyridylmethyl)amine and derivatives" Abstracts of Papers, 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-March 29, 2012 (2012), INOR-814.
- T. Baine, W. M. Singh, S. Kudo, N. J. DeYonker, T. C. Pham, D. L. Baker, C. E. Webster, X. Zhao. "Electrocatalytic and Photocatalytic Hydrogen Production from Water by a Molecular Pentacoordinated Cobalt Complex" Solar Fuels: Science, Engineering & Policy, Jan. 11-12, 2012, hosted by Duke University and the Solar Energy Research Center (SERC) at UNC-Chapel Hill (<http://www.serc.unc.edu/conf/>)

- H. Duan, T. C. Pham, D. L. Baker, C. E. Webster, X. Zhao, H. Zhou, J. C. Bollinger, B. Yan, Z. Wu, S. Tian, Y. Lu. "Synthesis, characterization, and reactivity of Mn complex with DPA-Bpy ligand" *Solar Fuels: Science, Engineering & Policy*, Jan. 11-12, 2012, hosted by Duke University and the Solar Energy Research Center (SERC) at UNC-Chapel Hill (<http://www.serc.unc.edu/conf/>)
- S. Kudo, W. M. Singh, T. Baine, N. DeYonker, C. E. Webster, X. Zhao. "Thermodynamic Study of Hydrogen Evolution from Water by Mononuclear Pentacoordinated Cobalt Complex" *Solar Fuels: Science, Engineering & Policy*, Jan. 11-12, 2012, hosted by Duke University and the Solar Energy Research Center (SERC) at UNC-Chapel Hill (<http://www.serc.unc.edu/conf/>)
- T. K. Hollis, X. Zhang, A. M. Wright, N. J. DeYonker, N. I. Hammer, C. E. Webster, E. J. Valente. "Synthesis, air-stability, photo-bleaching, and DFT modeling of blue light-emitting platinum CCC-N-heterocyclic carbene pincer complexes" Abstracts, 63rd Southeast Regional Meeting of the American Chemical Society, Richmond, VA, United States, October 26-29 (2011), SERM-599.
- T. C. T. Pham, I. W. Wanjala, A. L. Howard, D. K. Breland, N. J. DeYonker, C. E. Webster, A. L. Parrill, D. L. Baker. "Characterizing the structure and function of lipid preferring nucleotide pyrophosphatase phosphodiesterases using computational and experimental methods" Abstracts, 63rd Southeast Regional Meeting of the American Chemical Society, Richmond, VA, United States, October 26-29 (2011), SERM-274.
- P. L. Ranaivo, S. J. Symes, J. D. Swan, C. E. Webster, P. S. Simone, G. L. Emmert. "Structural Determination of the Products from the Reaction of Haloacetic Acid with Nicotinamide in Drinking Water Analysis" PITTCON Conference and Expo 2011, Atlanta, GA, United States, March 13-18, 2011, Session 1870-7.
- T. J. Burkey, K. L. Mosley, C. E. Webster, K. R. Ruddick, P. P. Lubet, J. O. Johnson, E. J. Heilweil. "Photochromic cyclopentadiene manganese tricarbonyl derivatives: Participation of imine group during linkage isomerization" Abstracts of Papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010, INOR-652.
- K. L. Mosley, K. R. Ruddick, J. O. Johnson, C. E. Webster, T. J. Burkey. "Synthesis of new photochromic organometallics based on a linkage isomerization" Abstracts of Papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010, INOR-567.
- X. Zhao, R. Grudzien, J. A. Ivie, K. R. Ruddick, C. E. Webster. "Water oxidation by ruthenium complexes with tris(2-pyridylmethyl)amine derivatives" Abstracts of Papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010, FUEL-83.
- P. P. Kannam, R. Grudzien, J. A. Ivie, K. R. Ruddick, C. E. Webster, X. Zhao. "Design of Ru Complexes for Water Oxidation" 33rd Annual Area Collegiate Chemistry Meeting, Apr. 10, 2010, hosted by the University of Tennessee at Martin
- X. Zhao, R. Grudzien, J. Ivie, K. R. Ruddick, C. E. Webster. "Design of Ru complexes for water oxidation" Abstracts of Papers, 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010, INOR-933.
- K. Camara, R. Letterman, C. E. Webster, X. Zhao. "Synthesis and characterization of Mn-Ca complexes for water oxidation" Abstracts of Papers, 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010, INOR-241.
- K. L. Mosley, K. Ruddick, C. E. Webster, E. J. Heilweil, T. J. Burkey. "Synthesis and Photochemistry of Novel Organometallics" Abstracts, 38th Great Lakes Regional Meeting of the American Chemical Society, Chicago, IL, United States, May 13-16, 2009, GLRM-227.
- E. J. Heilweil, K. Mosley, K. R. Ruddick, C. E. Webster, T. J. Burkey. "Photochromic cyclopentadienyl manganese tricarbonyl derivatives: Studies of linkage isomerization and ultrafast time resolved infrared spectroscopy" Abstracts of Papers, 237th ACS National Meeting, Salt Lake City, UT, United States, March 22-26, 2009, INOR-435.
- K. L. Mosley, K. Ruddick, C. E. Webster; E. J. Heilweil, T. J. Burkey. "Synthesis and Photochemistry of New Photochromic Organometallics" Abstracts, 60th Southeast Regional Meeting of the American Chemical Society, Nashville, TN, United States, November 12-15, 2008, SERM-409.
- K. L. Mosley, K. R. Ruddick, C. E. Webster, E. J. Heilweil, T. J. Burkey. "Synthesis and Photochemistry of New Photochromic Organometallics" Graduate student poster presentation at 2009 Undergraduate Research Conference.
- E. J. Heilweil, K. L. Mosley, C. E. Webster, K. Ruddick, T. J. Burkey. "Ultrafast Time Resolved Infrared Spectroscopy of Photochromic Cyclopentadienyl Manganese Tricarbonyl Derivatives" Abstracts, 60th Southeast Regional Meeting of the American Chemical Society, Nashville, TN, United States, November 12-15, 2008, SERM-106.
- S. Kumar, D. L. Watkins, D. K. Breland, C. E. Webster, T. Fujiwara. "Solvatochromism of a Unique Bispiropyran" International Symposium on Stimuli-Responsive Materials, Hattiesburg, MS, United States, October 28-30, 2008.
- M. B. Hall, C. E. Webster, S. D. Zaric. "Theoretical identification of the intermediates and the reaction mechanism in the carbon-hydrogen bond activation by the photochemically generated hydrotris(3,5-dimethylpyrazol-1-yl) borato carbonyl rhodium" Abstracts of Papers, 233rd ACS National Meeting, Chicago, IL, United States, March 25-29, 2007, INOR-1070.
- B. A. Vastine, C. E. Webster, M. B. Hall. "Theoretical Studies of Oxidative Addition/Reductive Elimination through Pt(II)/Pt(IV) Centers by Density Functional Theory." Abstracts, 60th Southwest Regional Meeting of the American Chemical Society, Fort Worth, TX, United States, September 29-October 4, 2004, SEPT04-066.
- C. Beddie, C. E. Webster, Y. Fan, M. B. Hall. "Density Functional Theory Investigations on the Mechanism of Urea Degradation Catalyzed by Urease Model Complexes." Abstracts, 60th Southwest Regional Meeting of the American Chemical Society, Fort Worth, TX, United States, September 29-October 4, 2004, SEPT04-456.
- C. E. Webster, M. Y. Darenbourg, P. A. Lindahl, M. B. Hall. "Structures and Energetics of Models for the Active Site of Acetyl-Coenzyme A Synthase: Role of Distal and Proximal Metals in Catalysis"—Poster presented at the 7th European Biological Inorganic Chemistry Conference (EUROBIC 7), Garmisch-Partenkirchen, Germany, August 29-September 2, 2004.
- C. E. Webster, M. B. Hall. "Separating Electronic, Steric, and Packing Interactions in Crystallographic Structures By Density Functional Theory"—Seminar presented at the Annual National Meeting of the American Crystallographic Association (ACA), Chicago, IL, July 17-22, 2004.

- Y. B. Fan, C. E. Webster, M. B. Hall. "Theoretical study on the mechanism of the regioselective functionalization of alkanes catalyzed by CpRh( $\eta^5$ -C<sub>5</sub>H<sub>5</sub>) complex." Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003, INOR-665, 225, U128.
- S. D. Zaric, C. E. Webster, M. B. Hall. "Theoretical study of alkane activation by tris (pyrazolyl)borate rhodium carbonyl." Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003, INOR-752, 225, U142.
- C. E. Webster, M. B. Hall. "Theoretical studies of inorganic and organometallic reaction mechanisms: Carbon-hydrogen and carbon-carbon bond activation of cyclopropane by cationic iridium(III) and neutral rhodium(I) and iridium(I) complexes." Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United States, August 18-22, 2002, INOR-013, 224, U642.
- C. E. Webster, M. B. Hall. "Predicting Structures and Energetics in Transition Metal Polyhydride Complexes"—Seminar presented at the XIX Congress and General Assembly of the International Union of Crystallography (IUCr), Geneva, Switzerland, August 6-15, 2002.
- M. B. Hall, C. E. Webster. "The theoretical transition state structure of a model complex bears a striking resemblance to the active site structure of DMSO reductase." Poster presented at the International Conference on Bioinorganic Chemistry (ICBIC) 10, Florence, Italy, August 26-31, 2001; *J Inorg Biochem* 2001, 86, 246.
- C. E. Webster, M. B. Hall. "Theoretical Studies of the Reaction Mechanism of Dimethylsulfoxide Reductase with Inorganic Model Complexes: Six vs. Seven Coordinate Reaction Mechanism and DMSO Coordination to the Active Site"—Poster presented at Molybdenum & Tungsten Enzymes, Gordon Research Conference, Queen's College, Oxford, England, July 1-6, 2001.
- C. E. Webster, M. B. Hall. "Structure and rearrangements of an Ir tris(pyrazolyl)borate tetrahydride complex"—Poster presented at EURO-Hydrides 2000, Universit  de Bourgogne, Dijon, France, September 6-9, 2000.
- C. R. Bowers, J. Bharatam, V. Storhaug, C. E. Webster, A. Cottone, R. Gianna, B. J. Gaffney. "Laser-polarized xenon-(129) NMR & BET isotherm analysis of Xe adsorption on lyophilized proteins." Platform presented at the Federation of American Societies for Experimental Biology (FASEB), Biophysical Society 43rd Annual Meeting, Baltimore, MD, February 13-17, 1999; *Biophys J* 1999, 76, A136.

#### CONTRIBUTED PRESENTATIONS BY GROUP MEMBERS

- L. Olive, E. Van Dornshuld, and C. E. Webster. "Curious case of DMSO: A computational study" Abstracts of Papers, 258th ACS National Meeting & Exposition, San Diego, CA, United States, August 25-29, 2019 (2019), COMP-0281.
- G. Liang, P. Wang, X. Zhao, C. E. Webster. "Theoretical Investigation on the Electronic and Steric Tuning of Catalytic H<sub>2</sub> Evolution by Cobalt Complexes" Feeding and Powering the World 2018: Planning for the Future, July 16-17, 2018, The University of Mississippi, Oxford, MS.
- M. Zhang, E. V. Dornshuld, J. C. Bunquin, M. Delferro, T. K. Hollis, C. E. Webster. "The Platinum Electronic Parameter (PtEP): A Compliment to TEP" Feeding and Powering the World 2018: Planning for the Future, July 16-17, 2018, The University of Mississippi, Oxford, MS.
- R. W. Lamb, C. E. Webster. "Update from the Webster Group" Feeding and Powering the World 2018: Planning for the Future, July 16-17, 2018, The University of Mississippi, Oxford, MS.
- V. A. K. Adiraju, B. Donnadieu, C. E. Webster, T. K. Hollis. "Early Transition Metal CCC-NHC Pincer Complexes" Feeding and Powering the World 2018: Planning for the Future, July 16-17, 2018, The University of Mississippi, Oxford, MS.
- K. Adiraju, M. Zhang, E. Dornshuld, R. W. Lamb, G. Liang, C. E. Webster, T. K. Hollis. "State-of-the-Art Nitrogen Reduction: Haber-Bosch to Homogeneous back to Heterogeneous" Feeding and Powering the World 2018: Planning for the Future, July 16-17, 2018, The University of Mississippi, Oxford, MS.
- H. Hessler, G. M. Lang, C. E. Webster, T. K. Hollis "Synthesis of next-generation CCC-NHC pincer backbones" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-1406.
- R. W. Lamb, A. Huckaba, H. Shirley, S. L. Guertin, S. Autry, H. Cheema, K. Talukdar, Jones, Tanya C.; J. W. Jurss, A. Antonysamy, N. Hammer, R. H. Schmehl, J. H. Delcamp, C. E. Webster "Photocatalyzed HER: A computational investigation on the mechanism of a novel, record-setting catalyst, (pyNHC-p-CF<sub>3</sub>Ph)W(CO)<sub>4</sub>" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-1305.
- T. K. Hollis, C. E. Webster, M. Zhang, E. V. Dornshuld, Bunquin, Jeffrey C.; Delferro, Massimiliano "NHC pincer complex donor ability? PtEP (platinum (Pt) electronic parameter): A donicity scale incorporating strictly meridional, tridentate ligands" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-595.
- G. Liang, C. E. Webster "Missing agostomer in the fluxionality of cyclohexenylmanganese tricarbonyl [(C<sub>6</sub>H<sub>9</sub>)Mn(CO)<sub>3</sub>]" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-199.
- E. V. Dornshuld, M. Zhang, T. K. Hollis, C. E. Webster "Characterizing 195Pt NMR chemical shifts with computationally tractable non-relativistic density functional approaches" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-198.
- V. Dixit, M. Zhang, E. V. Dornshuld, T. K. Hollis, C. E. Webster "Theoretical study of the effect of substituents on the optical spectra and 195Pt NMR shift of CCC-NHC Pt(II) complexes" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-197.
- G. M. Lang, J. Denny, V. Dixit, C. E. Webster, T. K. Hollis "Quest to break the oxo-wall: Oxidation of a CCC-NHC-Pt complex" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-58.
- J. Denny, R. W. Lamb, C. E. Webster, T. K. Hollis "The synthesis, characterization, and applications of CCC-NHC pincer complexes of rhodium" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-57.

- J. D. Cope, J. A. Denny, R. W. Lamb, C. E. Webster, T. K. Hollis. "CCC-NHC pincer iron complexes: Synthesis, characterization, and electrochemistry" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-56.
- M. Zhang, S. Autry, V. Dixit, J. A. Denny, N. Hammer, C. E. Webster, Hollis, T. Keith "Synthesis, characterization, and photophysics of CCC-NHC pincer platinum complexes" Abstracts, 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-55.
- J. A. Denny, R. W. Lamb, C. E. Webster, T. K. Hollis. "Synthesis and Characterization of Rhodium CCC-NHC Pincer Complexes" Feeding and Powering the World 2017: Building the Knowledge Base, June 19-20, 2017, The University of Mississippi, Oxford, MS.
- R. W. Lamb, A. J. Huckaba, H. Shirley, S. Guertin, S. Autry, H. Cheema, K. Talukdar, T. Jones, J. W. Jurs, A. Dass, N. I. Hammer, R. H. Schmehl, J. H. Delcamp, C. E. Webster. "New Insights into the Mechanism of the HER Catalyzed by (py-NHC-p-CF<sub>3</sub>Ph)W(CO)<sub>4</sub>" Feeding and Powering the World 2017: Building the Knowledge Base, June 19-20, 2017, The University of Mississippi, Oxford, MS.
- G. M. Lang, J. A. Denny, V. Dixit, C. E. Webster, T. K. Hollis. "Oxidation of a CCC-NHC Pt(II) Complex via O-atom Transfer Reactions" Feeding and Powering the World 2017: Building the Knowledge Base, June 19-20, 2017, The University of Mississippi, Oxford, MS.
- J. D. Cope, J. A. Denny, R. W. Lamb, L. E. McNamara, N. I. Hammer, C. E. Webster, T. K. Hollis. "Synthesis, Characterization, Photophysics, Ligand Rearrangement of CCC-NHC Pincer Nickel Complexes used for Electrocatalytic Reduction of CO<sub>2</sub>" Feeding and Powering the World 2017: Building the Knowledge Base, June 19-20, 2017, The University of Mississippi, Oxford, MS.
- T. R. Helgert, J. A. Denny, T. K. Hollis, and C. E. Webster. "CCC-NHC Pincer Ta Complexes: Synthesis and Reactivity" Feeding and Powering the World 2017: Building the Knowledge Base, June 19-20, 2017, The University of Mississippi, Oxford, MS.
- M. Zhang, E. V. Dornshuld, V. Dixit, J. A. Denny, C. E. Webster, T. K. Hollis. "Synthesis and Characterization of CCC-NHC Pincer Platinum Complexes" Feeding and Powering the World 2017: Building the Knowledge Base, June 19-20, 2017, The University of Mississippi, Oxford, MS.
- T. R. Helgert, J. A. Denny, G. M. Lang, G. Liang, C. E. Webster, T. K. Hollis. "Extreme  $\pi$ -loading as a design element for accessing imido reactivity: CCC-NHC Ta bis(imido) pincer complex synthesis and reactivity in oxidative amination" Abstracts of Papers, 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017 (2017), INOR-591.
- J. Cope, M. Zhang, T. K. Hollis, and C. E. Webster. "Synthesis and characterisation of CCC-NHC supported complexes containing group 10 metals" Feeding and Powering the World 2016: Building the Network, The University of Mississippi, Oxford, MS, July 25-26, 2016.
- V. Dixit, E. V. Dornshuld, and C. E. Webster. "Substitution effects on the emission spectra of Platinum CCC-NHC Pincer Complexes" Feeding and Powering the World 2016: Building the Network, The University of Mississippi, Oxford, MS, July 25-26, 2016.
- E. V. Dornshuld, M. Zhang, X. Zhang, T. K. Hollis, and C. E. Webster. "Utilizing computational <sup>195</sup>Pt NMR chemical shifts for the prediction of meridional ligand donor ability in square planar complexes" Feeding and Powering the World 2016: Building the Network, The University of Mississippi, Oxford, MS, July 25-26, 2016.
- R. W. Lamb, C. E. Webster, J. H. Delcamp. "Mechanistic Study of HER Catalyzed by a Novel W-NHC Complex" Feeding and Powering the World 2016: Building the Network, The University of Mississippi, Oxford, MS, July 25-26, 2016.
- M. Zhang, E. V. Dornshuld, X. Zhang, T. K. Hollis, C. E. Webster. "Predicting Metal Complex Reactivity for Energy Applications: Donicity of Meridional Tridentate Ligands: <sup>195</sup>Pt NMR of CCC-NHC Pt Pincer Square Planar Complexes" Feeding and Powering the World 2016: Building the Network, The University of Mississippi, Oxford, MS, July 25-26, 2016.
- T. Harrison, T. K. Hollis, C. E. Webster. "The general method of synthesizing 1,3-[3'-(trimethylsilylmethyl)-benzimidazole]benzene preligand pincer: Metalation and trans metalation of the three activated C-H bonds" Feeding and Powering the World 2016: Building the Network, The University of Mississippi, Oxford, MS, July 25-26, 2016.
- I. McCraw, T. K. Hollis, C. E. Webster. "Synthesis and Characterization of 1,3-bis(3'-(neohexyl)-imidazolyl)benzene Pincer Ligand with Subsequent Metalation and Platinum Transmetalation of Three Activated C-H Bonds" Feeding and Powering the World 2016: Building the Network, The University of Mississippi, Oxford, MS, July 25-26, 2016.
- R. Pearlman, J. Cope, T. K. Hollis, C. E. Webster. "The synthesis of light-emitting pincer CCC-bis(NHC) complexes" Feeding and Powering the World 2016: Building the Network, The University of Mississippi, Oxford, MS, July 25-26, 2016.
- T. Woodby, T. K. Hollis, C. E. Webster. "Synthesis, alkylation and metalation of bis CCC-NHC proligands" Feeding and Powering the World 2016: Building the Network, The University of Mississippi, Oxford, MS, July 25-26, 2016.
- E. V. Dornshuld, M. Zhang, X. Zhang, T. K. Hollis, C. E. Webster. "Predicting <sup>195</sup>Pt NMR chemical shifts in small Pt(II) and Pt(IV) organometallic compounds with density functional approaches" Abstracts, 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, United States, November 4-7 (2015), SERMACS-SWRM-360.
- R. W. Lamb, E. V. Dornshuld, C. E. Webster. "Computational investigation of linkage isomerization in sulfoxide-containing ruthenium complexes" Abstracts, 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, United States, November 4-7 (2015), SERMACS-SWRM-220.
- M. Zhang, X. Zhang, L. McNamara, N. Hammer, N. Kaneza, S. Pan, C. E. Webster, T. K. Hollis. "Synthesis, characterization, and luminescence of CCC-NHC pincer platinum complexes" Abstracts, 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, United States, November 4-7 (2015), SERMACS-SWRM-180.
- G. Liang, C. E. Webster. "Phosphoramidate hydrolysis catalyzed by hHINT1: A cluster-model DFT computational study" Abstracts, 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, United States, November 4-7 (2015), SERMACS-SWRM-19.



- G. Liang, C. E. Webster. "Phosphoramidate Hydrolysis Catalyzed by hHINT1: A Cluster-Model DFT Computational Study" Poster, 8th Mississippi Regional Biophysical Consortium, June 3-4, 2015, The University of Mississippi, Oxford, MS.
- C. Bernal, N. J. DeYonker, D. Rabinovich, C. E. Webster. "Using Electronic Structure Methods To Quantify Metal-Arene Bonding In Novel Pb-Centered Complexes" 89th Annual Florida Annual Meeting and Exposition, FAME 2013, Innisbrook, FL, May 9-11, 2013.
- K. N. Leigh, T. K. Hollis, C. E. Webster. "Catalytic intramolecular hydroamination by titanium(IV) and rhodium(III) CCC-NHC pincer complexes" Abstracts of Papers, 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013 (2013), INOR-1199.
- K. N. Leigh, J. P. Waltho, G.M. Blackburn, M. W. Bowler, C. E. Webster. "Computational studies of intermediate- and transition-state analogs in  $\beta$ -PGM" Abstracts of Papers, 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013 (2013), INOR-282.
- N. J. DeYonker, D. Isrow, A. Koppaka, B. Captain, C. E. Webster. "Metal - ligand synergistic effects in  $Ni(\eta^2\text{-TEMPO})_2$ , structures and reactivity" Abstracts of Papers, 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013 (2013), INOR-86.
- R. G. Letterman, C. B. Duke, T. T. To, T. J. Burkey, C. E. Webster. "How do inequivalent atoms in an organometallic complex become equivalent on the NMR timescale?" Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012 (2012), INOR-354.
- K. N. Leigh, T. K. Hollis, C. E. Webster. "Computational study of catalytic intramolecular hydroamination by a CCC-NHC Rh pincer complex" Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012 (2012), INOR-232.
- R. G. Letterman, N. J. DeYonker, T. J. Burkey, C. E. Webster. "Should density functional theory be used to guide the design of chromium-containing photochromic materials?" Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012 (2012), INOR-224.
- K. N. Leigh, J. P. Waltho, G. M. Blackburn, M. W. Bowler, C. E. Webster. "Utilization of computed  $^{19}\text{F}$  NMR to identify active site intermediate and transition-state analogs in  $\beta$ -PGM" Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012 (2012), INOR-55.
- N. J. DeYonker. "The Many Phosphoryl Transfers of Phospholipase D" Invited lecture, March 01, 2012, seminar presented at the University of Mississippi, Oxford, MS.
- J. A. Ivie, N. J. DeYonker, D. J. Darenbourg, C. E. Webster. "Theoretical Studies on the Mechanism of Copolymerization of Oxetane and Carbon Dioxide via (Salen)Chromium Catalysts" Abstracts, 63rd Southeast Regional Meeting of the American Chemical Society, Richmond, VA, United States, October 26-29 (2011), SERM-603.
- J. A. Ivie, D. J. Darenbourg, C. E. Webster. "Theoretical studies on the mechanism of copolymerization of oxetane and carbon dioxide via (salen)chromium catalysts" Abstracts of Papers, 241st ACS National Meeting, Anaheim, CA, United States, March 27-31, 2011, INOR-520.
- K. R. Ruddick, K. L. Mosley, J. O. Johnson, T. J. Burkey, C. E. Webster. "Computational design of organometallic photochromic systems of the type  $\text{CpMn}(\text{CO})_2\text{L}$  and  $\text{ArylCr}(\text{CO})_2\text{L}$  where L is a chelating, bifunctional tethered side-chain" Abstracts of Papers, 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010, INOR-834.
- J. A. Ivie, K. R. Ruddick, R. M. Grudzien, X. Zhao, C. E. Webster. "Computational approach to the design of ruthenium water oxidation catalysts" Abstracts of Papers, 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010, INOR-240.
- F. Greene, D. K. Breland, S. Kumar, T. Fujiwara, C. E. Webster. "Study on the thermodynamics behind the binding behavior of spiro form spirooxazine dimers" Abstracts of Papers, 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010, INOR-227.
- D. K. Breland, S. Kumar, T. Fujiwara, C. E. Webster. "Ring Opening and Isomerization Mechanisms in Spiropyran and Spirooxazine Dimers" Abstracts, 61st Southeast Regional Meeting of the American Chemical Society, San Juan, Puerto Rico, October 21-24, 2009, SRM-594.
- D. K. Breland, D. L. Baker, A. Parrill, C. E. Webster. "The Phosphoryl Transfer Mechanism in Xac Nucleotide Pyrophosphatase/Phosphodiesterase: A Computational Study" Abstracts, 61st Southeast Regional Meeting of the American Chemical Society, San Juan, Puerto Rico, October 21-24, 2009, SRM-449.
- K. Ruddick, K. L. Mosley, T. J. Burkey, C. E. Webster. "Computational Design of Organometallic Photochromic Systems" Abstracts, 38th Great Lakes Regional Meeting of the American Chemical Society, Chicago, IL, United States, May 13-16, 2009, GLRM-229.
- K. Ruddick, K. L. Mosley, T. J. Burkey, C. E. Webster. "Computational and Experimental Studies of Organometallic Photochromic Systems: Isomerization Mechanisms for Bifunctional Side-chain Complexes" Abstracts of Papers, 237th ACS National Meeting, Salt Lake City, UT, United States, March 22-26, 2009, INOR-670.
- D. K. Breland, D. L. Baker, A. L. Parrill, C. E. Webster. "Computational Model Reveals Intermediate in Catalytic Mechanism of Xac Nucleotide Pyrophosphatase/Phosphodiesterase" Abstracts, 60th Southeast Regional Meeting of the American Chemical Society, Nashville, TN, United States, November 12-15, 2008, SERM-137.
- D. Enekwa, C. E. Webster. "Computational study of catalysis of the 3-Aza-Cope rearrangement in a  $\text{Ga}_4\text{L}_6^{12-}$  supramolecular host" Abstracts, 62nd Southwest Regional Meeting of the American Chemical Society, Houston, TX, United States, October 19-22, 2006, SRM-419.
- J. M. Seat, C. E. Webster. "A Computational Investigation of the Mechanism of Ribosylhomocysteinease" 29th Annual Area Collegiate Chemistry Meeting, Martin, TN, April 29, 2006.