Thomas R. Cundari
Dept. of Chemistry
CASCaM
University of North Texas
Box 305070
Denton, TX 76203-5070
phone:940-369-7753
fax:940-565-4318
e-mail: t@unt.edu

Education:
- B. S.: Pace University, New York City (1986)
- Ph. D.: University of Florida (1990)

Academic Positions Held:
- Pace University: Laboratory Assistant (1984-1986)
- University of Florida: Graduate Teaching and Research Assistant (Sept. 1986- May. 1990); Major Professor: Russell S. Drago
- North Dakota State University: Post-Doctoral Research Associate (June 1990 - Aug. 1991); Collaborator: Mark S. Gordon
- University of Memphis: Assistant Professor (Aug. 1991 - Aug. 1995)
- University of Memphis: Associate Professor (Sept. 1995 – Aug. 2000)
- University of Memphis: Professor (Sept. 2000 – August 2002)
- Dunavant University Professorship (Sept. 2000 – August 2002)
- University of North Texas: Professor (Sept. 2002 – Aug. 2008)
- University of North Texas: Regents Professor (Sept. 2008 – present)
- Director, Center for Advanced Scientific Computing and Modeling, 2005 – present.

Visiting Scientist and Sabbatical Positions:
- Visiting Scientist, National Institutes of Standards and Technology/Center for Advanced Research in Biotechnology: (June 1992 - Sept. 1992); Collaborator: Walter J. Stevens
- Visiting Scientist, Air Force Summer Faculty Research Associate, Phillips Laboratory, Emerging Technologies, Edwards Air Force Base: (June 1993 - August 1993); Collaborators: Joe Lichtenhan and E. J. Wucherer
- Visiting Scientist and Workshop Speaker, Parallel Programming on the IBM SP1, Cornell Theory Center, Cornell University (April 1994)
- Visiting Scientist, Los Alamos National Laboratory (June - August 1994), Collaborator: Jeffrey C. Bryan.
- Visiting Scientist, Cornell Theory Center, Cornell University (Summer 1995)
- Professional Development Assignment, Theory-Experiment Study of Transition Metal/C-H Bond Interactions, University of Bristol (UK), Collaborator: Prof. A. Guy Orpen.
- NSF Scholar in Residence at NIH, Advanced Biomedical Computing Center, National Cancer Institute, (Feb – May 2001)

Editing and Advisory Council Activities:
- Advisory Council for the ACS journal *Journal of Chemical Information and Computational Sciences* (now called Journal of Chemical Information and Modeling), 2000 – 2005.
- Edited, "Computational Organometallic Chemistry" Marcel Dekker, Inc., New York, 2001.
- Co-Editor, "Reviews in Computational Chemistry;" Wiley, New York, 2002 – 2009.
- Editorial Board, *Computational and Theoretical Chemistry*, 2007 – present.
- Editorial Board, *Journal of Coordination Chemistry*, 2012 – present.
- Editorial Advisory Board for the ACS journal *Organometallics*, 2013 – present.
- Editorial Board, *Polyhedron*, 2013 – present.

Honors and Awards:
- Four-Year, Full Scholarship, Pace University (1982-1986)
- Top Chemistry Student at Pace University (1983,1984,1985,1986)
- Shell Foundation Fellowship for Top Fourth Year Graduate Student at the University of Florida (1990)
- Kickoff Speaker for National Chemistry Week at Arkansas State University

- Awarded Early Tenure and Promotion to Associate Professor, 1994.
- Early Career Research Award, University of Memphis, 1994.
- Superior Performance in University Research, University of Memphis, 1995.
- Top Poster Presentation, Small Molecules Indaba, South African Crystallographic Society, IUCr Commission on Small Molecules, Skukuza, South Africa, 1995.
- External Examiner for Ph. D. Dissertation, University of Calgary, Department of Chemistry, Nov. 1995.
- Superior Performance in University Research, University of Memphis, 1996.
- College of Arts & Sciences Distinguished Research Award, University of Memphis, 1998.
- Outstanding Paper Award, "Neural Networks in Inorganic Chemistry," Sigma Xi, Memphis Chapter, 1998
- Alumni Association Distinguished Research Award, University of Memphis, 2000.
- Dunavant University Professorship, University of Memphis (Sept. 2000 – August 2003)
- Decker Scholar, University of North Texas (Sept. 2007 – Sept. 2009)
- Doherty Award, DFW-ACS Local Section (2013)

Service:
- Faculty Search Committee, Analytical Chemistry: 1991 & 1992
- Departmental Equipment Committee: Sept. 1991 - May 1992
- Departmental Graduate Studies Committee: May 1992 – Aug. 2002
- Member, Faculty Research Grant Proposal Review Board, University of Memphis (Sept. 1993 - Sept. 1995)
- Faculty Evaluator for "Works in Progress" Symposium, Selection Committee for 1994 National Undergraduate Research Conference, University of Memphis (Nov. 94 -)
- Chairman, Awards Committee, Memphis Section of the American Chemical Society, 1994.
- Search Committee, Vice Provost for Research and the Graduate School, University of Memphis, 1994 - 1995.
- Lecturer, Unity in Science Day, Memphis City Schools, U of Memphis, Jan. 1996.
- Session Chairman, Symposium on Advances in Computational Inorganic Chemistry, 212th ACS National Meeting, Orlando, FL, August 1996.
- Co-organized (with Henry Kurtz and Abby Parrill) the 28th Southeast Theoretical Chemistry Association meeting, Memphis, TN, April 23 - 24, 1999.
- Symposium organizer, "Effective Core Potential Methods in Hartree-Fock and Density Functional Theory;" 220th ACS National Meeting, San Francisco, CA, Spring 2000.
- Coordinator, Chemistry Department NSF-REU Program, The University of Memphis, 2000 - 2002.
- Symposium organizer, "Computational Organometallic Chemistry;" 222nd ACS National Meeting, Chicago, IL, Summer 2001.
- Organizing Committee, 8th Electronic Computational Chemistry Conference, March 4 – April 1, 2002.
- Chair, Graduate Affairs Committee, Department of Chemistry, University of North Texas, Fall 2003 - 2006.
- Member and Chair, Search Committee, Welch Endowed Chair in Chemistry, Fall 2003 - Spring 2004 and Fall 2019 – Spring 2020, respectively.
- Symposium co-organizer (with Nikita Matsunaga), "Spin Forbidden and Open-Shell Processes;" 226th ACS National Meeting, New York, NY, Summer 2003.

Publications (Graduate School):
1 - "A Molecular Orbital Investigation of the Dissymmetry in Side-On Bonded Dioxygen Complexes;" T. R. Cundari, R. S. Drago, M. C. Zerner Inorg. Chem. **1988**, 26, 4239.
2 - "Structural and Energetic Analysis of Gas-Phase Ammonium Ions with Relevance to the 'Anomalous' Order in Amine Basicities;" T. R. Cundari, D. E. Ferris, R. S. Drago J. Org. Chem. **1989**, 54, 1042-1047.
3 - "Ru-Oxo Catalyzed Epoxidations and the Woodward-Hoffmann Rules;" T. R. Cundari, R. S. Drago Intern. J. Quantum Chem. **1989**, 36, 773-790.
4 - "A Molecular Orbital Investigation of Ru-Oxo Catalyzed Alcohol Oxidations;" T. R. Cundari, R. S. Drago Intern. J. Quantum Chem., Proc. 1989 Sanibel Symp. **1989**, 23, 489-499.
5 - "Utility of the Semi-Empirical INDO/1 Method for the Calculation of the Geometries of Second-Row Transition Metal Species;" W. P. Anderson, T. R. Cundari, R. S. Drago, M. C. Zerner Inorg. Chem. **1990**, 29, 1-3 (communication).
6 - "Molecular Orbital Investigation of Ru-Oxo Catalyzed Epoxidations;" T. R. Cundari, R. S. Drago Inorg. Chem. **1990**, 29, 487-497.

7 - "Molecular Orbital Investigation of the Oxidation of Olefins by Cis- and Trans-Ruthenium(VI)-Dioxo Complexes;" T. R. Cundari, R. S. Drago Inorg. Chem. **1990**, 29, 2303-2308.

8 - "Oxidation of Alcohols by Six-Coordinate Ru(IV)-Oxo Complexes;" T. R. Cundari, R. S. Drago Inorg. Chem. **1990**, 29, 3904-3907.

9 - "Alkane Hydroxylations;" T. R. Cundari, R. S. Drago Intern. J. Quantum Chem., Proc. 1990 Sanibel Symp. **1990**, 24, 665-678.

10 - "An Intermediate Neglect of Differential Overlap Model for Second Row Transition Metal Species;" W. P. Anderson, T. R. Cundari, M. C. Zerner Intern. J. Quantum Chem. **1991**, 39, 31- 45.

Publications (Post-Doctoral Work):

11 - "Principal Resonance Contributors to High-Valent, Transition-Metal Alkylidene Complexes;" T. R. Cundari, M. S. Gordon J. Am. Chem. Soc. **1991**, 113, 5231-5243.

12 - "Theoretical Investigations of Olefin Metathesis Catalysts;" T. R. Cundari, M. S. Gordon Organometallics **1992**, 11, 55-63.

13 - "A Comparative Study of the Bonding in Heteroatom Analogues of Benzene;" M. W. Schmidt, N. Matsunaga, T. R. Cundari, M. S. Gordon Theor. Chim. Acta **1992**, 83, 57-68 (invited).

14 - "The Nature of the Transition Metal-Silicon Double Bond;" T. R. Cundari, M. S. Gordon J. Phys. Chem. **1992**, 96, 631-636.

15 - "Further Investigations of High-Valent, Transition Metal Alkylidene Complexes;" T. R. Cundari, M. S. Gordon J. Am. Chem. Soc. **1992**, 114, 539-548.

16 - "Strategies for Designing High-Valent, Transition Metal Silylidene Ligands;" T. R. Cundari; M. S. Gordon Organometallics **1992**, 11, 3122-3129.

17 - "The Electronic Structure of Transition Metal Disilene Complexes;" T. R. Cundari; M. S. Gordon, "Recent Advances in Computational Silicon Chemistry" special issue of J. Mol. Struct. **1994**, 313, 47-54 (invited).

Publications: (University of Memphis)

18 - "The Activation and Elimination of H_2 by Zr Complexes;" T. R. Cundari Intern. J. Quantum Chem., Proc. Sanibel Symp. **1992**, 26, 793-806.

19 - "Transition Metal Imido Complexes;" T. R. Cundari J. Am. Chem. Soc. **1992**, 114, 7879-7888.

20 - "Methane Activation by Group IVB Imido Complexes;" T. R. Cundari J. Am. Chem. Soc. **1992**, 114, 10557-10663.

21 - "Effective Core Potential Methods for the Lanthanides;" T. R. Cundari; W. J. Stevens J. Chem. Phys. **1993**, 98, 5555-5565.

22 - "A Structural and Computational Study of Tetraaqua[2,6-Diacetylpyridine bis(semicarbazone)] gadolinium(III) trinitrate;" S. O. Sommerer; B. L. Westcott; T. R. Cundari; J. Krause Inorg. Chem. Acta **1993**, 209, 101 - 104 (communication).

23 - "Small Molecule Elimination from Group IVB Amido Complexes;" T. R. Cundari; M. S. Gordon J. Am. Chem. Soc. **1993**, 115, 4210 - 4217.

24 - "Methane Adducts of d^0, Transition Metal Complexes;" T. R. Cundari Organometallics **1993**, 12, 1998 - 2000 (communication).

25 - "Effective Core Potential Study of Transition and Lanthanide Metal Catalyzed Hydrogen Exchange;" T. R. Cundari; S. O. Sommerer; W. J. Stevens Chem. Phys. **1993**, 178, 235 - 243.

26 - "C-H Activation by a d^2 W-imido Complex: Comparison of [2+2] and Oxidative Addition Pathways;" T. R. Cundari Organometallics **1993**, 12, 4971 - 4978.

27 - "The Reactions of Co^+ (^3F-d^8) with H_2 and CH_4;" N. Koga, J. Musaev, K. Morokuma, T. R. Cundari, K. A. Nguyen; M. S. Gordon J. Phys. Chem. **1993**, 97, 11435 - 11444.

28 - "Calculation of a Methane C-H Oxidative Addition Trajectory: Comparison to Experiment and Methane Activation by High-Valent Complexes.;" T. R. Cundari J. Am. Chem. Soc. **1994**, 116, 340 - 347.

29 - "Rhenium-Oxo-Bis(acetylene) Anions: Structure, Properties, and Electronic Structure. Comparison of Re-O Bonding with That in Other Rhenium-Oxo Complexes;" T. R. Cundari; S. C. Critchlow; R. R. Conry; E. Spaltenstein; K. A. Hall; S. Tahmassebi, J. M. Mayer Organometallics **1994**, 13, 322 - 331.

30 - "An Effective Core Potential Study of Transition Metal Chalcogenides. Part I. Molecular Structure;" M. T. Benson, T. R. Cundari, S. J. Lim, H. D. Nguyen, K. Pierce-Beaver J. Am. Chem. Soc. **1994**, 116, 3955 - 3966.

31 - "Effective Core Potential Study of Multiply Bonded Transition Metal Complexes of the Heavier Main Group Elements;" M. T. Benson, T. R. Cundari, Y. Li, L. A. Strohecker Intern. J. Quantum Chem., Proc. Sanibel Symp. **1994**, 28, 181 - 194.

32 - "Quantum Modeling of Lanthanide Complexes on Parallel Supercomputers;" T. R. Cundari; L. A. Strohecker Proc. 1994 Scalable High Performance Computing Conference **1994**, 710 - 717.

33 - "Methane Activation by Group VB Bis(Imido) Complexes;" T. R. Cundari Organometallics **1994**, 13, 2987 - 2994.

34 - "Effective Core Potential Studies of Transition Metal Chemistry;" T. R. Cundari; M. S. Gordon Coord. Chem. Rev. **1996**, 147, 87 - 115.

35 - "Applications of Parallel GAMESS;" K. K. Baldridge; J. A. Boatz; T. R. Cundari; M. S. Gordon; J. H. Jensen; N. Matsunaga, M. W. Schmidt, T. L. Windus. American Chemical Society Symposium Series 592, Mattson, T. G. (Ed.), ACS: Washington, D. C., **1995**, chapter 3 (invited).

36. "Effects of "π-Loading" in Technetium tris(Imido) Complexes;" J. C. Bryan; A. K. Burrell; M. T. Benson; T. R. Cundari; J. Barrera; K. A. Hall in "Technetium in Chemistry and Nuclear Medicine," M. Nicolini, G. Bandoli and U. Mazzi (Eds.) SGE Ditoriali, Padova, **1995**.

37 - "Bonding and Structure of Heavily π-loaded Complexes;" M. T. Benson; J. C. Bryan, A. K. Burrell, T. R. Cundari Inorg. Chem. **1995**, 34, 2348 - 2355.

38 - "H_2 Elimination and Activation by Group IVA-Group IVB Complexes;" T. R. Cundari; Y. Li Int. J. Quantum Chem. **1995**, 55, 315 - 328.

39 - "Effective Core Potential Methods for the Lanthanides: The Trihalides;" T. R. Cundari, S. O. Sommerer, L. A. Strohecker, L. Tippett J. Chem. Phys. **1995**, 103, 7058 - 7063.

40 - "Methane Activation by Tris(Imido) Complexes: The Effect of Metal, Charge and d Orbital Occupation;" M. T. Benson; T. R. Cundari; E. W. Moody "Aspects of C-H Activation" special issue of J. Organomet. Chem. (Crabtree, R. H., Ed.) **1995**, 504, 1 - 13 (invited).

41 - "Effective Core Potential Approaches to the Chemistry of the Heavier Elements;" M. T. Benson, T. R. Cundari, M. L. Lutz, S. O. Sommerer "Reviews in Computational Chemistry;" D. Boyd; K. Lipkowitz (Eds.) **1996**, 8, 145 - 202 (invited).

42 - "Computer Aided Design of Metallopharmaceuticals: A Molecular Mechanics Force Field for Gadolinium Complexes;" T. R. Cundari; E. W. Moody, S. O. Sommerer Inorg. Chem. **1995**, 34, 5989 - 5999.

43 - "Decomposition Pathways for a Model TiN Chemical Vapor Deposition Precursor;" T. R. Cundari; J. M. Morse Chem. Mater **1996**, 8, 189 - 196.

44 - "Substituent Effects on Methane Activation and Elimination by High-Valent Zr Complexes;" T. R. Cundari, S. Curtiss Intern. J. Quantum Chem. **1996**, 60, 779 - 788.

45 - "X-ray Diffraction without X-rays: Modern Approaches to Organometallic Chemistry;" ACA Transaction Symposium - T. R. Cundari, E. S. Ignarra, E. W. Moody, P. D. Raby, S. O. Sommerer **1995**, 31, 23 - 30 (invited).

46. - "Activation and Elimination of Methane and Larger Hydrocarbons;" T. R. Cundari, N. Matsunaga, E. W. Moody J. Phys. Chem. **1996**, 100, 6475 - 6483.

47 - "A Molecular Mechanics Force Field for Platinum(II) Coordination Complexes;" T. R. Cundari, W. Fu, E. W. Moody, L. L. Slavin, L. A. Snyder, S. O. Sommerer; T. R. Klinckman J. Phys. Chem. **1996**, 100, 18057 - 18064.

48 - "Catalytic Alkane Dehydrogenation;" M. T. Benson; T. R. Cundari in "Metal Hydrogen Bonding" special issue of Inorg. Chim. Acta (U. Bellucco, Ed.) **1997**, 259, 91 - 100 (invited).

49 - "A Comparison of Neural Networks and Quantum Mechanics for Inorganic Systems;" T. R. Cundari, E. W. Moody J. Chem. Info. Comput. Sci. **1997**, 37, 871 - 875.

50 - "Conformational Analysis of Platinum Antitumor Drugs;" T. R. Cundari, W. Fu J. Mol. Struct. (THEOCHEM) **1998**, 425, 51 - 60.

51 - "Methane Activation by Mercury(II) Complexes;" T. R. Cundari, A. Yoshikawa J. Comp. Chem. **1998**, 19, 902 - 908.

52 - "Synthesis, Structure, Computational Studies and Magnetic Properties of a Ten-Coordinate Gadolinium Complex;" M. T. Benson, T. R. Cundari, L. C. Saunders, S. O. Sommerer Inorg. Chim. Acta **1997**, 258, 127 - 130 (communication).

53 - "Electrostatic-Covalent Model Parameters for Molecular Modeling;" T. R. Cundari, R. S. Drago, in Computational Thermochemistry, American Chemical Society Symposium Series, K. K. Irikura; D. J. Frurip (Eds.), ACS: Washington, D. C., **1997**, pp. 105 - 118 (invited).

54 - "Theoretical Estimation of Vibrational Frequencies Involving Transition Metal Compounds;" T. R. Cundari, P. D. Raby J. Phys. Chem. A **1997**, 101, 5783 - 5788.

55 - "Quantum Modeling of the Chemical Vapor Deposition of Transition Metal Materials;" T. R. Cundari, S. O. Sommerer Advanced Materials **1997**, 9, 183 - 192.

56- "Reaction Pathways for Model II-VI Precursors. A Computational Study;" T. R. Cundari , W. Fu Intern. J. Quantum Chem. **1999**, 71, 47 - 56.

57 - "Molecular Modeling of Vanadium Peroxides;" T. R. Cundari, L. L. Sisterhen, C. L. Stylianopoulos Inorg. Chem. **1997**, 36, 4029 - 4034.

58 - "Late Transition Metal Multiple Bonding. Platinum Phosphinidenes and Ruthenium Alkylidenes;" M T. Benson, T. R. Cundari Intern. J. Quantum Chem. **1997**, 65, 987 - 996.

59 - "Molecular Modeling of Vanadium Oxo Complexes. A Comparison of Quantum and Classical Methods;" T. R. Cundari, L. C. Saunders, L. L. Sisterhen J. Phys. Chem. **1998**, 102, 997 - 1004.

60 - "Prediction of Bond Dissociation Energies using Neural Network, Statistical, and Quantum Mechanical Approaches;" T. R. Cundari, E. W. Moody J. Mol. Struct. (THEOCHEM) **1998**, 425, 43 - 50.

61 - "Ligand and Substituent Effects in Methane Activation by Mercury(II) Complexes;" T. R. Cundari, L. A. Snyder, A. Yoshikawa J. Mol. Struct. (THEOCHEM) **1998**, 425, 13 - 24.

62 - "Modeling Lanthanide Coordination Complexes. Comparison of Semiempirical and Classical Methods;" T. R. Cundari, L. C. Saunders J. Chem. Info. Comput. Sci. **1998**, 38, 523 - 528.

63 - "Rhodocenium Complexes Bearing the 1,2,3-Tri-tert-butylcyclopentadienyl Ligand: Redox-Promoted Synthesis and Mechanistic, Structural and Computational Investigations;" B. T. Donovan-Merkert, C. R. Clontz, L. M. Rhinehart, H. I. Tijong, C. M. Carlin, T. R. Cundari, A. L. Rheingold, I. Guzei Organometallics **1998**, 17, 1716 - 1724.

64 - "Cyclometalation of Alkylphosphines;" M. T. Benson, T. R. Cundari in "Intermolecular Interactions, Proceedings of The Structural Chemistry Indaba II;" Gans, W.; Boeyens, J. C. A., Eds. Plenum: New York, **1998**, pp. 71 - 81.

65 - "Modeling Nonlinear Optical Properties of Transition Metal Complexes. Basis Set, Effective Core Potential and Geometry Effects;" T. R. Cundari, H. A. Kurtz, T. Zhou J. Phys. Chem. A **1998**, 102, 2962 - 2966.

66 - "A Structural Dichotomy in 6-Coordinate d Complexes: Trigonal Prismatic $(^{t}BuSiC{\equiv}C)_6Ta^{-}$ and Octahedral $(^{t}Bu_3SiC{\equiv}C)_6Zr^{2-}$;" T. P. Vaid, A. S. Veige, E. M. Lobkovsky, W. V. Glassey, P. T. Wolczanski, L. M. Liable-Sands, A. L. Rheingold, T. R. Cundari J. Am. Chem. Soc. **1998**, 120. 10067 - 10079.

67 - "Molecular Modeling of d- and f-Block Metal Complexes;" T. R. Cundari J. Chem. Soc., Dalton **1998**, 2771 - 2776 (invited).

68 - "Reduced Variation Space Analysis of Methane Adducts;" T. R. Cundari, T. R. Klinckman Inorg. Chem. **1998**, 37, 5399 - 5401.

69 - "PM3(tm) Analysis of Transition Metal Complexes;" T. R. Cundari, J. Deng J. Chem. Info. Comput. Sci. **1999**, 39, 376 - 381.

70 - "Modeling Nonlinear Optical Properties of Inorganic Complexes. Counterion Effects;" T. R. Cundari, H. A. Kurtz, T. Zhou Chem. Phys. **1999**, 240, 205 - 214.

71 - "Molecular Modeling of Catalysts and Catalytic Reactions;" T. R. Cundari, J. Deng, W. Fu, T. R. Klinckman, A. Yoshikawa J. Chem. Info. Comput. Sci. **1998**, 38, 941 - 948.

72 - "Multiple Bonding in Transition Metal Complexes;" T. R. Cundari Chem. Rev. **2000**, 100, 807 - 818 (invited).

73 - "Late Transition Metal Multiple Bonding: The Case of a Silver(III)-Oxo Complex;" T. R. Cundari, W. Fu, J. N. Harvey, T. R. Klinckman Inorg. Chem. **1999**, 38, 5611 - 5615.

74 - "Genetic Algorithm Optimization of Semiempirical Parameters for Transition Metals;" T. R. Cundari, J. Deng, W. Fu Intern. J. Quantum Chem. **2000**, 77, 421 - 432. (invited, Zerner Festschrift).

75 - "Genetic Algorithm Optimization of a Molecular Mechanics Force Field for Technetium;" T. R. Cundari, W. Fu Inorg. Chem. Acta **2000**, 300 - 302, 113 - 124 (invited).

76 - "A Computational Study of Polarizabilities and Second Hyperpolarizabilities of Inorganic Transition Metal Thiometalates and Metalates in Solution", T. R. Cundari; H. A. Kurtz; T. Zhou J. Phys. Chem. A. **2000**, 104, 4711 - 4717 special issue on "Electronic and NLO Materials - Theory and Modeling"

77 - "Soft Computing Techniques for Mining Structural Databases;" T.R. Cundari, J. Deng, H. F. Pop, C. Sârbu J. Chem. Info. Comput. Sci. **2000**, 40, 1052 - 1061.

78 - "Database Mining using Soft Computing Techniques. An Integrated Neural Network-Fuzzy Logic-Genetic Algorithm Approach;" T. R. Cundari, M. Russo J. Chem. Info. Comput. Sci. **2001**, 41, 281 – 287.

79 - "Intermolecular Effects on Nonlinear Optical Properties of Inorganic Complexes. An Effective Core Potential Study;" T. R. Cundari, H. A. Kurtz, T. Zhou J. Chem. Info. Comp. Sci. **2001**, 41, 38 - 42, special issue on "Effective Core Potentials in Hartree Fock and Density Functional Theory"

80 - "Inter- and Intramolecular Experimental and Calculated Equilibrium Isotope Effects for $(silox)_2(^{t}Bu_3SiND)TiR$ + RH (silox = $^{t}Bu_3SiO$); Inferred Kinetic Isotope Effects for RH/D Addition to Transient $(silox)_2Ti{=}NSi^{t}Bu_3$" L. M. Slaughter, P. T. Wolczanski, T. R. Klinckman, T. R. Cundari J. Am. Chem. Soc. **2000**, 122, 7953 – 7975.

81 - "Synthesis, Molecular Structure and Computational Study of a Ruthenium Bis(thietane) Complex;" P. M. Nave, M. Draganjac, B. Ward, A. W. Cordes, T. M. Barclay, T. R. Cundari, J. J. Carbo, F. Maseras Inorg. Chim. Acta. **2001**, 316, 13 – 18.

82 - "Kinetics of Substitution of Weakly Coordinating Nitrate by Chloride in (η^5-Cp)Ru(CO)(ER_3)ONO_2 (ER_3 = $AsPh_3$, PPh_3, P(p-anisyl)$_3$, PPh_2(o-anisyl), P(OPh)$_3$) in Dichloromethane;" M. Cao, V. Liem, N. W. Hoffman, M. L. Kwan, J. K. Little, J. M. McGilvray, C. B. Morris, B. C. Soderberg, A. Wierzbicki, T. R. Cundari, C. M. Lake, E. A. Valente Organometallics **2001**, *20*, 2270 – 2279.

83 - "Deoxygenations of (silox)$_3$WNO and R$_3$PO by (silox)$_3$M (M = V, Ta) and (silox)$_3$NbL (silox = ^{t}Bu$_3$SiO): Consequences of Electronic Effects;" A. S. Veige, L. M. Slaughter, P. T. Wolczanski, N. Matsunaga, S. A. Decker, T. R. Cundari J. Am. Chem. Soc. **2001**, 123, 6419 – 6420. (communication).

84 - "A Combined Genetic Algorithm - Neural Network Optimization of a Propane Ammoxidation Catalyst;" T. R. Cundari, J. Deng, Y. Zhao Ind. Eng. Chem. **2001**, 40, 5475 – 5480.

85 - "DFT Study of the Ethylene Hydroformylation Catalytic Cycle Employing a HRh(PH_3)$_2$(CO) Model Catalyst;" T. R. Cundari, S. A. Decker Organometallics **2001**, 20, 2827 - 2841.

86 - "Cooperative Stepwise Reduction of N_2 by a Low-Coordinate Iron Complex;" J. M. Smith, R. J. Lachicotte, K. R. Rodgers, G. Lukat-Rodgers, K. A. Pittard, T. R. Cundari, P. L. Holland J. Am. Chem. Soc. **2001**, 123, 9222 – 9223. (communication)

87- "Hybrid QM/MM Study of Propene Insertion into the Rh-H bond of HRh(PPh_3)$_2$(CO)(η^2-CH_2=$CHCH_3$): The Role of the Olefin Adduct in Determining Product Selectivity" T. R. Cundari, S. A. Decker J. Organomet. Chem. **2001**, 635, 132 – 141. (invited) Special Issue Celebrating the 50th Anniversary of Dewar-Chatt-Duncanson theory.

88 - "A Quantum Mechanics/Molecular Mechanics Study of the Steric Influence of the PR_3 Spectator Ligands on the Energetics of Ethylene Insertion into the Rh-H bond of HRh(PR_3)$_2$(CO)(η^2-CH_2=CH_2);" T. R. Cundari, S. A. Decker New J. Chem. **2002**, 26, 129 – 135.

89 - "Carbon-Hydrogen Bond Activation by Titanium Imidos. Computational Evidence for the Role of Alkane Adducts in Selective C-H Activation;" T. R. Cundari, T. R. Klinckman, P. T. Wolczanski J. Am. Chem. Soc. **2002**, 124, 1481 - 1487.

90 - "De Novo Structural Prediction of Transition Metal Complexes. Application to Technetium;" C. Buda, S. K. Burt, T. R. Cundari, P. S. Shenkin Inorg. Chem. **2002**, 41, 2060 – 2069.

91 - "Can Semi-Empirical Quantum Mechanics Be Used to Predict the Spin State of Transition Metal Complexes? An Application of De Novo Prediction;" D. M. Ball, C. Buda, T. Cundari, A. M. Gillespie, D. P. White Inorg. Chem. **2002**, 41, 152 – 156.

92 - "Novel Transition Metal Multiple Bonding...Myth or Reality? A Computational Investigation of Boryl Complexes;" T. R. Cundari, Y. Zhao Inorg. Chim. Acta **2003**, 345, 70 – 80 (invited) Special Schrock issue.

93 - "Robust Fuzzy Principal Component Analysis (FPCA). A Comparative Study Concerning Interaction of Carbon-Hydrogen with Molybdenum Oxo Bonds;" T. R. Cundari, H. F. Pop, C. Sarbu J. Chem. Info. Comp. Sci. **2002**, 42, 1363 – 1369.

94 - "Semiempirical Quantum Mechanics and the Quantification of Ligand Electronic Parameters;" T. R. Cundari, A. M. Gillespie, K. A. Pittard, D. P. White Int. Elec. J. Mol. Design **2002**, 1, 242 - 251 (invited, special Randić issue).

95 - "Electronically Unsaturated Chloride and Methyl Complexes of Iron, Cobalt, and Nickel;" P. L. Holland, T. R. Cundari, L. L. Perez, N. A. Eckert, R. J. Lachicotte J. Am. Chem. Soc. **2002**, 124, 14416 - 14424.

96 - "A Priori Assessment of the Stereoelectronic Profile of Phosphine and Phosphites;" K. D. Cooney, T. R. Cundari, N. W. Hoffman, K. A. Pittard, M. D. Temple, Y. Zhao J. Am. Chem. Soc. **2003**, 125, 4318 - 4324.

97 - "Computational Study of Methane Activation by TpRe(CO)$_2$ and CpRe(CO)$_2$ with a Stereoelectronic Comparison of Cyclopentadienyl and Scorpionate Ligands;" R. G. Bergman, T. R. Cundari, T. B. Gunnoe, A. G. Gillespie, W. D. Harman, T. R. Klinckman, M. D. Temple, D. P. White Organometallics **2003**, 22, 2331-2337.

98 - "Direct Solution of Schrodinger Equation by a Parallel Genetic Algorithm;" R. Saha, S. P. Bhattacharyya, C. D. Taylor, Y. Zhao, T. R. Cundari Intern. J. Quantum Chem. **2003**, 94, 243-250.

99 - "ONIOM Study of the Active Species in Pd-phosphine Catalyzed Coupling Reactions;" Cundari, T. R.; Deng, J.; Zhao, Y. J. Mol. Struct. (THEOCHEM), **2003**, 732, 121-129 (invited, special issue on QM/MM Calculations in Biology and Chemistry, Ruiz-Lopez, M. F., Ed.).

100 - "Olefin Insertion and Subsequent β-X Elimination from a Pentacoordinate Tantalum Complex. A Density Functional Theory Study;" T. R. Cundari and C. D. Taylor Organometallics **2003**, 22, 4047-4059.

101 - "Symmetry and Geometry Considerations of Atom Transfer: Deoxygenations of $(silox)_3WNO$ and R_3PO (R = Me, Ph, tBu) by $(silox)_3$(M (M = V, NbL (L = PMe_3, 4-picoline), Ta; silox = $^tBu_3SiO$);" A. S. Veige, L. M. Slaughter, E. M. Lobkovsky, P. T. Wolczanski, N. Matsunaga, S. A. Decker, T. R. Cundari Inorg. Chem. **2003**, 42, 6204-6224.

102 - "Gas-Phase Ligand Substitution in a Square-Planar Rh(I) Complex via a Dissociative Rather than Associative Pathway: an ESI FT-ICR MS and DFT Investigation;" R. E. Bossio, T. R. Cundari, N. W. Hoffman, A. G. Marshall Organometallics **2004**, 23, 144-148.

Publications: (University of North Texas)

103 - "Jahn-Teller Distortion in the Phosphorescent Excited State of Three-coordinate Au(I) Phosphine Complexes;" K. A. Barakat, T. R. Cundari, M. A. Omary J. Am. Chem. Soc. **2003**, 125, 1428-14229. (communication).

104 - "Synthesis and Reactivity of a Coordinatively Unsaturated Ru(II) Parent Amido Complex: Studies of X-H Activation (X = H or C);" D. Conner, K. N. Jayaprakash, T. R. Cundari, T. B. Gunnoe Organometallics **2004**, 23, 2724-2733.

105 - "Function of Conserved Residues of Human Glutathione Synthetase: Implications for the PreATP Grasp Superfamily;" A. Dinescu, V. Bhansali, J. Luo, T. R. Cundari, M. E. Anderson J. Biol. Chem. **2004**, 279, 22412-22421.

106 - "Carbon-hydrogen and Carbon-heteroatom Bond Activation using Iridium (I) Complexes;" T. R. Cundari, S. Vaddadi Inorg. Chim. Acta **2004**, 357, 2863-2869.

107- "Experimental and Computational Studies of Ru(II) Catalyzed Addition of Arene C-H Bonds to Olefins;" M. Lail, C. M. Bell, T. R. Cundari, D. Conner, T. B. Gunnoe, J. L. Petersen Organometallics **2004**, 23, 5007-5020.

108 - "Reversible Beta-Hydrogen Elimination: Rearrangement and Thermodynamics of Three-Coordinate Iron(II) Alkyl Complexes;" J. Vela, T. R. Cundari, S. Vaddadi, J. M. Smith, E. A. Gregory, R. J. Lachicotte, P. L. Holland Organometallics **2004**, 23, 5226 - 5239.

109 - "Reaction of TpRu(CO)(NCMe)(Me) (Tp = hydridotris(pyrazolyl)borate) with Heteroaromatic Substrates: Stoichiometric and Catalytic C-H Activation;" K. A. Pittard, J. P. Lee, T. R. Cundari, T. B. Gunnoe, J. L. Petersen Organometallics **2004**, 23, 5514-5523.

110 - "De Novo Prediction of Ground State Multiplicity and Structural Isomerism for Transition Metal Complexes;" C. Buda, T. R. Cundari J. Mol. Struct., THEOCHEM **2004**, 686, 137 - 145.

111 - "Calculation of the Enthalpies of Formation for Transition Metal Complexes;" T. R. Cundari, H. A. Ruiz Leza, T. Grimes, G. A. Steyl, A.Waters, A. K. Wilson Chem. Phys. Lett **2005**, 401, 58 - 61.

112 - "Chemical and Photophysical Properties of Au^I, Au^{II}, Au^{III}, and Au^I-Dimer Complexes;" K. A. Barakat, T. R. Cundari Chem. Phys. **2005**, 311, 3-11.

113 - "Conversions of Ru(III) Alkyl Complexes to Ru(II) Complexes Through Ru-C_{alkyl} Bond Homolysis;" M. Lail, T. B. Gunnoe, K. A. Barakat, T. R. Cundari Organometallics **2005**, 24, 1301 - 1305.

114 - Density Functional Theory Study of Palladium Catalyzed Aryl-Nitrogen and Aryl-Oxygen Bond Formation T. R. Cundari, J. Deng J. Phys. Org. Chem. **2005**, 18, 417 - 425.

115 - "Low Coordinate Chromium Siloxides: the "Box" $[(\mu\text{-Cl})Cr(\mu\text{-OSi}^tBu_3)]_4$, Distorted Trigonal $[(^tBu_3SiO)_3Cr][Na(benzene)]$ and $[(^tBu_3SiO)_3Cr][Na(dibenzo\text{-}18\text{-}c\text{-}6)]$, and Trigonal $(^tBu_3SiO)_3Cr$;" O. L. Sydora, P. T. Wolczanski, E. B. Lobkovsky, C. Buda, T. R. Cundari Inorg. Chem. **2005**, 44, 2606-2618.

116 - "Thermodynamics, Kinetics and Mechanism of $(silox)_3M$(olefin) to $(silox)_3M$(alkylidene) Rearrangements (silox = $^tBu_3SiO$; M = Nb, Ta);" K. F. Hirsekorn, A. S. Veige, M. P. Marshak, Y. Koldobskaya, P. T. Wolczanski, T. R. Cundari, E. B. Lobkovsky J. Am. Chem. Soc. **2005**, 127, 4809-4830.

117 - "De Novo Prediction of the Ground State Structure of Transition Metal Complexes using Semiempirical and Ab Initio Quantum Mechanics. Coordination Isomerism;" C. Buda, T. R. Cundari, A. A. Flores J. Coord. Chem. **2005**, 58, 575 - 585.

118 - "N-Heterocyclic Carbenes of the Late Transition Metals: A Computational and Structural Database Study;" E. Baba, T. R. Cundari, I. Firkin Inorg. Chim. Acta **2005**, 358, 2867 - 2875. Shepherd special issue. (6/1/04)

119 - "Ground State Prediction of Linkage Isomerism for Transition Metal Complexes using Quantum Mechanics;" C. Buda, A. Dinescu, A. B. Kazi, T. R. Cundari - J. Chem. Info. Model. **2005**, 45, 965 - 970.

120 - "Monomeric Thallium(I) Complexes of Fluorinated Triazapentadienyl Ligands;" H. V. R. Dias, S. Singh, T. R. Cundari Angew. Chem. **2005**, 44, 4907 - 4910 (communication).

121 - "Electronic Features of $[(silox)_2Mo{=}NR]_2(\mu\text{-Hg})$: 3-Center-4-Electron Bonding Controls Reactivity, While its Frontier Orbitals are Key to Estimating a Dimolybdenum π-Bond Strength;" D. C. Rosenfeld, K.

Barakat, C. Buda, P. T. Wolczanski, T. R. Cundari J. Am. Chem. Soc. **2005**, 127, 8262 - 8263 (communication).

122 - "Effect of the Coinage Metal on the Electronic Energy and Electrostatic Potential of Luminescent Trinuclear Pyrazolate Ring Complexes;" T. R. Cundari, H. V. Rasika Dias, H. V. Diyabalanage, O. Elbjeirami, M. A. Gonser, T. Grimes, M. A. Omary, M. Rawashdeh-Omary Inorg. Chem. **2005**, 44 8200 - 8210 (cover article).

123 - "Evidence for the Net Addition of Arene C-H Bonds Across a Ru(II)-Hydroxide Bond;" Y. Feng, M. Lail, K. A. Barakat, T. R. Cundari, T. B. Gunnoe, J. L. Petersen J. Am. Chem. Soc. **2005**, 127, 14174-14175 (communication).

124 - "Synthesis of the Five-Coordinate Ruthenium(II) Complexes [(PCP)Ru(CO)(L)][BAr'$_4$] (PCP = 2,6-($CH_2P^tBu_2$)$_2C_6H_3$, BAr'$_4$ = 2,6-(CF_3)$_2C_6H_3$, L = η^1-$ClCH_2Cl$, η^1-N_2, or μ-Cl-Ru(PCP)(CO)): Reactions with Phenyldiazomethane and Phenylacetylene;" J. Zhang, K. A. Barakat, T. R. Cundari, T. B. Gunnoe, P. D. Boyle, J. L. Petersen, C. S. Day;" Inorg. Chem. **2005**, 44, 8379-8390.

125 - "Ruthenium(II)-Mediated Carbon-Carbon Bond Formation between Acetonitrile and Pyrrole: Combined Experimental and Computational Study;" K. A. Pittard, T. R. Cundari, T. B. Gunnoe, C. S. Day, J. L. Petersen Organometallics **2005**, 24, 5015-5024.

126 - "A T-shaped Three-Coordinate Nickel(I) Carbonyl Complex and the Geometric Preferences of Three-Coordinate d^9 Complexes;" N. A. Eckert, A. Dinescu, T. R. Cundari, P. L. Holland Inorg. Chem. **2005**, 44, 7702-7704 (communication).

127 - "Studies of N_2 Fixation at Low-Coordinate Iron Complexes;" J. M. Smith, A. R. Sadique, T. R. Cundari, K. R. Rodgers, G. Lukat-Rodgers, R. J. Lachicotte, C. J. Flaschenreim, J. Vela, P. L. Holland J. Am. Chem. Soc. **2006**, 128, 756-769.

128 - "Bidentate Coordination of Pyrazolate in Low-Coordinate Iron(II) and Nickel(II) Complexes;" J. Vela, S. Vaddadi, S. Kingsley, C. J. Flaschenriem, R. J. Lachicotte, T. R. Cundari, P. L. Holland Angew. Chem., Int. Ed. **2006**, 45, 1607 - 1611 (communication).

129 - "The Butterfly Dimer [(^{t}Bu$_3$SiO)Cr]$_2$(μ-OSi^{t}Bu$_3$)$_2$ and Its Oxidative Cleavage to (^{t}Bu$_3$SiO)$_2$Cr(=N-N=CPh$_2$)$_2$ and (^{t}Bu$_3$SiO)$_2$Cr=N(2,6-Ph$_2$-C_6H_3);" O. L. Sydora, D. S. Kuiper, P. T. Wolczanski, E. B. Lobkovsky, A. Dinescu, T. R. Cundari Inorg. Chem. **2006**, 45, 2008 - 2021.

130 - "Oxygen Atom Transfer Enthalpies. Assessment of the Effect of Method and Solvent;" A. Dinescu, R. Combs, C. Whiteley, T. R. Cundari J. Phys. Chem. A. **2006**, 110, 4053-4056.

131 - "Carbon-Hydrogen versus Carbon-Heteroatom Activation by a High-Valent Zirconium-Imido Complex;" T. R. Cundari, A. W. Pierpont, H. Rabaâ Intern. J. Quantum Chem. **2006**, 106, 1611-1619.

132 - "Reactions of a Ru(II) Phenyl Complex with Substrates that Possess C-N or C-O Multiple Bonds: C-C Bond Formation, N-H Bond Cleavage and Decarbonylation Reactions;" J. P. Lee, K. A. Pittard, N. DeYonker, T. R. Cundari, T. B. Gunnoe, J. L. Petersen Organometallics **2006**, 25, 1500-1510.

133 - "The Correlation-Consistent Composite Approach (ccCA): An Alternative to the Gaussian-n Methods;" N. J. DeYonker, T. R. Cundari, A. K. Wilson J. Chem. Phys. **2006**, 124, 114104/1-17.

134 - Intertrimer and Intratrimer Metallophilic and Excimeric Bonding in the Ground and Phosphorescent States of Trinuclear Coinage Metal Pyrazolates: A Computational Study;" T. Grimes, M. A. Omary, H. V. Rasika Dias, T. R. Cundari J. Phys. Chem. A **2006**, 110, 5823 - 5830.

135 - "Hydrogen-Deuterium Exchange between TpRu(PMe$_3$)(L)X (L = PMe$_3$ and X = OH, OPh, Me, Ph, or NHPh; L = NCMe and X = Ph) and Deuterated Arene Solvents: Evidence for Metal-Mediated Processes;" Y. Feng, M. Lail, N. A. Foley, T. B. Gunnoe, K. A. Barakat, T. R. Cundari, J. L. Petersen J. Am. Chem. Soc. **2006**, 128, 7982-7994.

136 - "Disproportionation of Gold(II) Complexes. A Density Functional Theory Study;" T. R. Cundari, K. A. Barakat, H. Rabaâ, M. A. Omary J. Phys. Chem. B **2006**, 110, 14645 – 14651.

137 - "Accurate Enthalpies of Formation of Alkali and Alkaline Earth Metal Oxides and Hydroxides: An Assessment of the Correlation Consistent Composite Approach (ccCA);" D. S. Ho, N. J. DeYonker, A. K. Wilson, T. R. Cundari J. Phys. Chem A **2006**, 110, 9767 - 9770.

138 - "Single-Electron Oxidation of Monomeric Copper (I) Alkyl Complexes: Evidence for Reductive Elimination through Bimolecular Formation of Alkanes;" L. A. Goj, E. D. Blue, S. A. Delp, T. B. Gunnoe, T. R. Cundari, J. L. Petersen Organometallics **2006**, 25, 4097 - 4104.

139 – "The correlation-consistent Composite Approach (ccCA): Application to the G3/99 Test Set;" N. J. DeYonker, T. Grimes, S. M. Yockel, A. Dinescu, B. J. Mintz, T. R. Cundari, A. K. Wilson J. Chem. Phys. **2006**, 125, 104111/1-15.

140 - "Hydrogen Atom Abstraction by an Fe(III) Imido Intermediate;" N. A. Eckert, S. Vaddadi, S. Stoian, C. J. Flaschenriem, T. R. Cundari, E. Munck, P. L. Holland Angew. Chem, Int. Ed. **2006**, 45, 6868 – 6871. (communication).

141 - "Chemistry Surrounding Monomeric Copper(I) Methyl, Phenyl, Anilido, Ethoxide and Phenoxide Complexes Supported by *N*-Heterocyclic Carbene Ligands;" L. A. Goj, E. D. Blue, S. A. Delp, T. B. Gunnoe, T. R. Cundari, A. W. Pierpont, J. L. Petersen, P. D. Boyle Inorg. Chem. **2006**, 45, 9032 – 9045.

142 - "Theoretical Study of Group Transfer from Multiply Bonded Nickel Complexes to Ethylene;" T. R. Cundari, S. Vaddadi J. Mol. Struct. THEOCHEM **2006**, 801, 47- 53.

143 - "Octahedral $[TpRu(PMe_3)_2OR]^{n+}$ Complexes (Tp = hydridotris(pyrazolyl)borate; R = H or Ph; n = 0 or 1): Reactions at Ru(II) and Ru(III) Oxidation States with Substrates that Possess Carbon-Hydrogen Bonds;" Y. Feng, T. B. Gunnoe, T. V. Grimes, T. R. Cundari Organometallics **2006**, 25, 5456 – 5465.

144 - "Calculation of Gas-Phase Enthalpies of Formation with Chemical Accuracy. The Curious Case of 3-Nitroaniline;" N. J. DeYonker, T. R. Cundari, A. K. Wilson, C. Sood, D. H. Magers J. Mol. Struct. THEOCHEM **2006**, 775, 77 – 80.

145 - "The Application of Modern Computational Chemistry Methods to Organometallic Systems;" in Comprehensive Organometallic Chemistry III, Volume 1 (Fundamentals), section 1.23, Crabtree, R. H.; Mingos, D. M. P. (Eds.) Elsevier: Oxford, **2006**, pp. 639 – 670. (invited).

146 - "A Molecular Modeling Study on the Enantioselectivity of Aryl Alkyl Ketone Reductions by a NADPH-dependent Carbonyl Reductase;" T. R. Cundari, A. Dinescu, D. Zhu, L. Hua J. Mol. Mod. **2007**, 13, 685 – 690.

147 - "Evidence for Strong Tantalum to Boron Dative Interactions in $(silox)_3Ta(BH_3)$ and $(silox)_3Ta(\eta^2\text{-B,Cl-}BCl_2Ph)$ (silox = $^tBu_3SiO$);" J. B. Bonanno, T. P. Henry, P. T. Wolczanski, A. W. Pierpont, T. R. Cundari Inorg. Chem. **2007**, 46, 1222 - 1232.

148 - "Catalytic Conversion of Nitroaromatics to Aryl Isocyanates by Copper Complexes. A Computational Study;" A. B. Kazi, T. R. Cundari, E. Baba, N. J. DeYonker, A. Dinescu, L. Spaine Organometallics **2007**, 26, 910 –914.

149 - "Catalytic Loop Motion in Human Glutathione Synthetase. A Molecular Modeling Approach;" A. Dinescu, M. E. Anderson, T. R. Cundari Biochem. Biophys. Res. Comm. **2007**, 353, 450 - 456.

150 - "Reactivity of TpRu(L)(NCMe)R (L = CO, PMe_3; R = Me, Ph) Systems with Isonitriles: Experimental and Computational Studies Toward the Intra- and Intermolecular Hydroarylation of Isonitriles;" J. P. Lee, J. -O. C. Jimenez-Halla, T. R. Cundari, T. B. Gunnoe J. Organomet. Chem. **2007**, 692, 2175 - 2186.

151 - "Comparative Reactivity of TpRu(L)(NCMe)Ph (L = CO or PMe_3): Impact of Ancillary Ligand L on Activation of Carbon-Hydrogen Bonds including Catalytic Hydroarylation and Hydrovinylation/Oligomerization of Ethylene;" N. A. Foley, M. Lail, J. P. Lee, T. B. Gunnoe, T. R. Cundari, J. L. Petersen J. Am. Chem. Soc. **2007**, 129, 6765 - 6781.

152 - "Computational Study of Methane Functionalization by a Multiply Bonded, Ni-bis(Phosphine) Complex;" T. R. Cundari, A. W. Pierpont, S. Vaddadi, J. Organomet. Chem. (Erker Special Issue) **2007**, 692, 4551 – 4559 (invited).

153 - "Activation of Carbon-Hydrogen Bonds via 1,2-Addition across M-X (X = OH or NH_2) Bonds of d^6 Transition Metals as a Potential Key Step in Hydrocarbon Functionalization: A Computational Study;" T. R. Cundari, T. V. Grimes, T. B. Gunnoe J. Am. Chem. Soc. **2007**, 129, 13172 - 13182.

154 – "Combined Experimental and Computational of $TpRu\{P(pyr)_3\}(NCMe)Me$ (pyr = N-pyrrolyl): Inter- and Intramolecular Activation of C-H Bonds and the Impact of Sterics on Catalytic Hydroarylation of Olefins;" N. A. Foley, M. Lail, T. B. Gunnoe, T. R. Cundari, P. D. Boyle, J. L. Petersen Organometallics **2007**, 26, 5507 - 5516.

155 - "Computational s-block thermochemistry with the correlation consistent Composite Approach and G3" N. J. DeYonker, D. S. Ho, A. K. Wilson, T. R. Cundari J. Phys. Chem. A **2007**, 111, 10776 - 10780.

156 – "Performance of the correlation-consistent Composite Approach (ccCA) for transition states: A comparison to G3B theory;" T. V. Grimes, T. R. Cundari, A. K. Wilson, N. J. DeYonker J. Chem. Phys. **2007**, 127, 154117/1-8.

157 - "Quantitative Computational Thermochemistry of Transition Metal Complexes;" T. R. Cundari, N. J. DeYonker, K. A. Peterson, G. Steyl, A. K. Wilson J. Phys. Chem. A **2007**, *111*, 11269-11277.

158 - "Synthesis and Reactivity of $[(silox)_2Mo{=}NR]_2Hg$: Unusual Thermal Stability and Ready Nucleophilic Cleavage Rationalized by Electronic Factors;" D. C. Rosenfeld, K. Barakat, C. Buda, P. T. Wolczanski, T. R. Cundari Inorg. Chem. **2007**, 46, 9715 – 9735.

159 - "Combined Experimental and Computational Studies on the Nature of Aromatic C-H Activation by Octahedral Ru(II) Complexes: Evidence for σ-Bond Metathesis from Hammett Studies;" N. J. DeYonker, N. A. Foley, T. R. Cundari, T. B. Gunnoe, J. L. Petersen Organometallics **2007**, *26*, 6604-6611.

160 - Synthesis and characterization of the first gold(I)-tris(ethylene) complex: $[Au(C_2H_4)_3][SbF_6]$;" H. V. R. Dias, M. Fianchini, T. R. Cundari, C. F. Campana Angew. Chem., Int. Ed. **2008**, 47, 556 - 559. (communication)

161 – Activation of sp^3 Carbon-Hydrogen Bonds by a Ru(II) Complex and Subsequent Metal-Mediated C-C and C-N Bond Formation;" N. A. Foley, T. B. Gunnoe, T. R. Cundari, P. D. Boyle, J. L. Petersen Angew. Chem., Int. Ed. **2008**, 47, 726 – 730. (communication)

162 - "Rational Design of Macrometallocyclic Trinuclear Complexes with Superior π Acidity and Basicity;" S. M. Tekarli, T. R. Cundari, M. A. Omary J. Am. Chem. Soc. **2008**, 130, 1669 – 1675.

163 - "Olefin Substitution in $(silox)_3M(olefin)$ (silox = $^tBu_3SiO$; M = Nb, Ta): The Role of Density of States in 2nd vs. 3rd Row Transition Metal Reactivity;" K. F. Hirsekorn, E. B. Hulley, P. T. Wolczanski, T. R. Cundari J. Am. Chem. Soc. **2008**, 130, 1183 - 1196.

164 - "Application of the correlation consistent Composite Approach (ccCA) to third row (Ga – Kr) molecules;" N. J. DeYonker, B. J. Mintz, T. R. Cundari, A. K. Wilson J. Chem. Theor. Comp. **2008**, 4, 328 – 334.

165 – "The Reactivity Patterns of Low-Coordinate Iron Hydride Complexes;" Y. Yu, A. R. Sadique, J. M. Smith, T. R. Dugan, T. R. Cundari, W. W. Brennessel, C. J. Flaschenriem, E. Bill, P. L. Holland J. Am. Chem. Soc. **2008**, 130, 6624 - 6638.

166 - "Aromatic C-H Activation and Catalytic Hydrophenylation of Ethylene by $TpRu\{P(OCH_2)_3CEt\}(NCMe)Ph$;" N. A. Foley, Z. Ke, T. B. Gunnoe, T. R. Cundari, J. L. Petersen Organometallics **2008**, 27, 3007 - 3017.

167 - "Molybdenum and Tungsten Structural Differences 6 are Dependent on $nd_{z2}/(n+1)s$ Mixing: Comparisons of $(silox)_3MX/R/$ (M = Mo, W; silox = $^tBu_3SiO$);" D. S. Kuiper, R. E. Douthwaite, A. R. Mayol, P. T. Wolczanski, E. B. Lobkovsky, T. R. Cundari, O. P. Lam, K. Meyer Inorg. Chem. **2008**, 47, 7139 – 7153.

168 - "Low Coordinate, Monomeric Molybdenum and Tungsten(III) Complexes: Structure, Reactivity and Calculational Studies of $(silox)_3ML$ (M = Mo, W; L = PMe_3, CO; silox = $^tBu_3SiO$);" D. S. Kuiper, P. T. Wolczanski, E. B. Lobkovsky, T. R. Cundari J. Am. Chem. Soc. **2008**, 130, 12931-12943.

169 - "Catalytic Tuning of Phosphinoethane Ligands for Improved C-H Activation;" T. R. Cundari, S. Vaddadi O. C. Jimenez-Halla, G. R. Morello J. Am. Chem. Soc. **2008**, 130, 13051-13058.

170 - "Bonding and Structure of Copper-Nitrenes;" T. R. Cundari, A. Kazi, A. Dinescu Inorg. Chem. **2008**, 47, 10067 - 10072.

171 - "Four-Coordinate Mo(II) as $(silox)_2Mo(PMe_3)_2$ and its W(IV) Congener $(silox)_2HW(\eta^2\text{-}CH_2PMe_2)(PMe_3)$ (silox = $^tBu_3SiO$);" D. S. Kuiper, P. T. Wolczanski, E. B. Lobkovsky, T. R. Cundari Inorg. Chem. **2008**, 47, 10542-10553.

172 - "Copper Nitrenes in Catalytic C-H Amination;" Y. M. Badiei, A. Dinescu, X. Dai, R. M. Palomino, F. Heinemann, T. R. Cundari, T. H. Warren Angew. Chem., Int. Ed. **2008**, 47,9961 - 9964.

173 - "Redox-Activation of Alkene Ligands in Platinum Complexes with Noninnocent Ligands;" J. L. Boyer, T. R. Cundari, N. J. DeYonker, T. B. Rauchfuss, S. R. Wilson Inorg. Chem. **2009**, 48, 638 - 645.

174 - "Sandwiched Sodium and Half-sandwiched Copper Carbonyl Complexes Featuring Polyfluorinated Tris(triazolyl)borate $[HB(3,5\text{-}(CF_3)_2Tz)_3]^-$;" Kou, X.; Wu, J.; Cundari, T. R.; Dias, H. V. R. J. Chem. Soc. Dalton **2009**, 915 - 917.

175 - "Arylpalladium Phosphonate Complexes as Reactive Intermediates in Phosphorus-Carbon Bond Forming Reactions;" M. C. Kohler, T. V. Grimes, X. Wang, T. R. Cundari, R. A. Stockland Jr. Organometallics **2009**, 28, 1193 - 1201.

176 - "Luminescence, Structural, and Bonding Trends upon Varying the Halogen in Isostructural Aurophilic Dimers;" O. Elbjeirami, M. A. Gonser, T. R. Cundari, M. A. Omary, B. N. Stewart, A. E. Bruce, M. R. M. Bruce Dalton Trans. **2009**, 1522 - 1533.

177 - "Coinage Metal-Ethylene Complexes Supported by Tris(pyrazolyl)borates: A Computational Study;" A. B. Kazi, H1. V. R. Dias, S. M. Tekarli, G. R. Morello, T. R. Cundari Organometallics **2009**, 28, 1826-1831.

178 - "Six-, Five- and Four-Coordinate Ruthenium(II) Hydride Complexes Supported by N-Heterocyclic Carbene Ligands: Synthesis, Characterization, Fundamental Reactivity and Catalytic Hydrogenation of Olefins, Aldehydes and Ketones J. P. Lee, Z. Ke, M. A. Ramírez, T. B. Gunnoe, T. R. Cundari, P. D. Boyle, J. L. Petersen Organometallics **2009**, 28, 1758-1775.

179 - "A Non-Classical Copper Carbonyl on a Tri-alkene Hydrocarbon Support;" M. Fianchini, T. R. Cundari, N. J. DeYonker, H. V. R. Dias Dalton Trans. **2009**, 2085-2087.

180 - "Unusual Electronic Features and Reactivity of the Dipyridylazaallyl Ligand: Characterization of $(smif)_2M$ (M = Fe, Co, Co^+, Ni; smif = $\{(2\text{-py})CH\}_2N$) and $[(TMS)_2NFe]_2(smif)_2$;" B. A. Frazier, P. T. Wolczanski, E. B. Lobkovsky, T. R. Cundari J. Am. Chem. Soc. **2009**, 131, 3428-3429. (communication).

181 - "Combined Experimental and Computational Study of W(II), Ru(II), Pt(IV), and Cu(I) Amine and Amido Complexes Using ^{15}N NMR Spectroscopy;" S. A. Delp, C. Munro-Leighton, N. M. Alsop, T. B. Gunnoe, T. R. Cundari, C. Khosla, J. L. Templeton J. Organomet. Chem. **2009**, 694, 1549-1556.

182 - "Ru(II) Catalysts Supported by Hydrido-tris(pyrazolyl)borate for the Hydroarylation of Olefins: Reaction Scope, Mechanistic Studies and Guides for the Development of Improved Catalysts;" N. A. Foley, J. P. Lee, Z. Ke, T. B. Gunnoe, T. R. Cundari Acc. Chem. Res. **2009**, 42, 585-597 (invited).

183 - "The Enthalpy of Formation of the Cyclohexadienyl Radical and the C-H Bond Enthalpy of 1,4-Cyclohexadiene: An Experimental and Computational Re-evaluation;" P. Marshall, E. C. Garrett, N. J. DeYonker, A. K. Wilson, T. R. Cundari J. Phys. Chem. A **2009**, 113, 6955 – 6963.

184 - "Combined Tight Binding/DFT Investigation of the Electronic Structure of Triimine-Platinum(II)/TCNQ Extended Stacks: Theoretical Prediction of Metallic Behavior;" H. Rabaâ, T. R. Cundari, M. A. Omary Can. J. Chem. (Ziegler Special Issue) **2009**, 87, 775 – 783 (invited).

185 - "Towards the Intrinsic Error of the correlation consistent Composite Approach (ccCA)", N. J. DeYonker, B. R. Wilson, T. G. Williams, A. W. Pierpont, T. R. Cundari, A. K. Wilson Mol. Phys. **2009**, 107, 1107 – 1121 (Schaefer special issue).

186 - "Accurate Thermochemistry for Transition Metal Complexes from First-Principles Calculations;" N. J. DeYonker, T. G. Williams, A. E. Imel, T. R. Cundari, A. K. Wilson J. Chem. Phys. **2009**, 131, 024106.

187 - "Cobalt-Dinitrogen Complexes With Weakened N-N Bonds;" K. Ding, A. W. Pierpont, W. W. Brennessel, G. Lukat-Rodgers, K. R. Rodgers, T. R. Cundari, P. L. Holland J. Am. Chem. Soc. **2009**, 131, 9471 - 9472 (communication).

188 - "Performance of Density Functional Theory for 3d Transition Metals-Containing Complexes: Utilization of the Correlation Consistent Basis Sets;" S. Tekarli, M. L. Drummond, T. G. Williams, T. R. Cundari, A. K. Wilson J. Phys. Chem. **2009**, 113, 8607 - 8614.

189 - "A Computational Study of Metal-Mediated Decomposition of Nitrene Transfer Reagents;" T. R. Cundari, G. R. Morello J. Org. Chem. **2009**, 74, 5711 – 5714.

190 - "Molecular DFT Structure and Packing Effect of Thiodipropionic and Dithiodiglycolic Acids and Salts;" H. Rabaâ, A. Ennaciri, T. R. Cundari, M. A. Omary;" C. Fan Journal of Molecular Structure: THEOCHEM **2009**, 911, 52 – 57.

191 - "Group-Transfer Reactions of Nickel-Carbene and -Nitrene Complexes with Organoazides and Nitrous Oxide that Form New C=N, C=O, and N=N Bonds;" N. D. Harrold, R. Waterman, G. L. Hillhouse, T. R. Cundari J. Am. Chem. Soc. **2009**, 131, 12872-12873.

192 - "CO_2-formatics: How Do Proteins Bind Carbon Dioxide?;" T. R. Cundari, A. K. Wilson, M. L. Drummond, H. E. Gonzalez, K. R. Jorgensen, S. Payne, J. Braunfeld, M. De Jesus, V. M. Johnson J. Chem. Info. Model. **2009**, 49, 2111-2115.

193 - "Activation of Carbon-Hydrogen and Hydrogen-Hydrogen Bonds by Copper-Nitrenes. A Comparison of Density Functional Theory and Composite Ab Initio Methods;" S. Tekarli, T. R. Cundari J. Comp. Theor. Chem. **2009**, 5, 2959 – 2966.

194 - "The correlation consistent Composite Approach (ccCA): Efficient and pan-periodic Kinetics and Thermodynamics;" T. R. Cundari, N. J. DeYonker, A. K. Wilson in "Advances in the Theory of Atomic and Molecular Systems Conceptual and Computational Advances in Quantum Chemistry;" Volume 19, P. Piecuch, J. Maruani, G. Delgado-Barrio, S. Wilson (Eds.) Springer: Netherlands, **2009**, pp. 197 – 224, (invited).

195 - "Palladium-Catalyzed C-H Activation/C-N Bond Formation Reactions: DFT Study of Reaction Mechanisms and Reactive Intermediates;" Z. Ke, T. R. Cundari Organometallics **2010**, 29, 821 - 834.

196 - "Periodic and Molecular Modeling Study of Donor-Acceptor Interactions in (dbbpy)Pt(tdt)•(TENF) and $[Pt(dbbpy)(tdt)]_2$•(TENF);" B. Chilukuri, Rabaâ, T. R. Cundari, J. M. Hudson, M. A. Omary, C. Minot Organometallics **2010**, 29, 795 – 800.

197 - "Towards Greener Carbon Capture Technologies: A Pharmacophore-Based Approach to Predict CO_2 Binding Sites in Proteins;" M. L. Drummond, T. R. Cundari, A. K. Wilson Energy & Fuels **2010**, 24, 1464 - 1470.

198 - "Determination of the Active Site of Sphingomonas chlorophenolica 2,6-dichloro-p-hydroquinone dioxygenase (PcpA);" T. E. Machonkin, P. L. Holland, K. N. Smith, J. S. Liberman, A. Dinescu, T. R. Cundari, S. S. Rocks J. Biol. Inorg. Chem. **2010**, 15, 291 – 301.

199 - "Computational Study of Methane C-H Activation with First-Row Late Transition Metal (M: Fe, Co, Ni) L_nM=E Catalysts;" T. R. Cundari, A. W. Pierpont Inorg. Chem. **2010**, 49, 2038 – 2046.

200 - "Modified Embedded Atoms Method (MEAM) Study of the Mechanical Properties of Carbon Nanotube Reinforced Nickel Composites;" J. Uddin, T. R. Cundari, A. K. Wilson, S. G. Srinivasan, M. I. Baskes Phys. Rev. B **2010**, 81, 104103/1-12. FA8650-08-C-5226

201 - "Net Hydrogenation of Pt-NHPh Bond Is Catalyzed by Elemental Pt;" J. R. Webb, A. W. Pierpont, C. Munro-Leighton, T. B. Gunnoe, T. R. Cundari, P. D. Boyle J. Am. Chem. Soc. **2010**, 132, 4520 - 4521 (communication).

202 - "Computational and Experimental Studies of Methyl Group Exchange Between Palladium(II) Centers;" M. S. Remy, T. R. Cundari, M. S. Sanford Organometallics **2010**, 29, 1522-1525.

203 - "Copper-Catalyzed Phosphinidene Transfer to Ethylene, Acetylene and Carbon Monoxide: A Computational Study;" M. J. Amme, A. B. Kazi, T. R. Cundari International Journal of Quantum Chemistry **2010**, 110, 1702 - 1711.

204 – "Theoretical Studies on the Catalysis of the Reverse Water Gas Shift Reaction Using First-row Transition Metal β-diketiminato Complexes;" C. Liu, L. Munjanja, T. R. Cundari, A. K. Wilson J. Phys. Chem. A **2010**, 114, 6207 – 6216.

205 - "Three-Coordinate Terminal Imidoiron(III) Complexes: Structure, Spectroscopy, and Mechanism of Formation;" R. E. Cowley, N. A. Eckert, N. J. DeYonker, C. Flaschenriem, T. R. Cundari, S. DeBeer George, E. Bill, P. L. Holland Inorg. Chem. **2010**, 49, 6172 – 6187.

206 - "Pnictogen-Hydride Activation by (silox)$_3$Ta (silox = ^{t}BuSiO); Attempts to Circumvent the Constraints of Orbital Symmetry in N_2 Activation;" E. B. Hulley, J. Bonanno, P. T. Wolczanski, T. R. Cundari, E. Lobkovsky Inorg. Chem. **2010**, 49, 8524 – 8544.

207 - "Structure and Dynamics of the Glycine Triad in Human Glutathione Synthetase;" M. E. Anderson, T. R. Cundari, S. Barelier, K. Slavens, T. Brown, A. Dinescu Biochem. Biophys. Res. Comm. **2010**, 400, 511 – 516. **1R15GM086833-01 (MEA)**

208 - "First-principle Study of Structure and Stability of Nickel Carbides;" J. S. Gibson, J. Uddin, T. R. Cundari, N. K. Bodiford, A. K. Wilson J. Phys. Condensed Matter **2010**, 22, 445503/1-7. **FA8650-08-C-5226**

209 - "Catalytic C-H Amination with Unactivated Amines via Copper(II) Amides;" S. Wiese, Y. M. Badiei, S. Mossin, R. T. Gephard, M. M. Melzer, M. S. Varonka, K. Meyer, T. R. Cundari, T. H. Warren Angew. Chem. **2010**, 49, 8850 - 8855. (communication).

210 - "Ligand Lone-Pair Influence on Hydrocarbon C-H Activation: A Computational Perspective;" D. H. Ess, T. B. Gunnoe, T. R. Cundari, W. A. Goddard III, R. A. Periana, T. J. Meyer Organometallics **2010**, 29, 6801 – 6815. **DE-SC0001298**

211 - Well-defined Copper(I) Amido Complex and Aryl Iodides Reacting to Form Aryl Amines;" S. A. Delp, L. A. Goj, C. Munro-Leighton, M. J. Pouy, J. P. Lee, T. B. Gunnoe, T. R. Cundari, J. L. Petersen Organometallics **2011**, 30, 55 - 57. (communication). **CHE-0701247**

212 - "A Two-Coordinate Nickel Imido Complex that Effects C–H Activation;" C A. Laskowski, A. J. M. Miller, G. L. Hillhouse, T. R. Cundari J. Am. Chem. Soc. **2011**, 133, 771-773. (communication). **DEFG02-03ER15387**

213 - "Modeling the Deposition of Metal Atoms on a p-Type Organometallic Conductor: Implications for Stability and Electron Transfer;" B. Chilukuri, T. R. Cundari J. Phys. Chem., C **2011**, 115, 5997 – 6003. **CHE-0911690**

214 - "Carbon Dioxide Reduction by Early Metal Compounds: A Propensity for Oxygen Atom Transfer;" V. A. Williams, D. R. Manke, P. T. Wolczanski, T. R. Cundari Inorg. Chim. Acta **2011**, 369, 203 – 214. (invited) (Bergman Special Issue). **BER-08ER64603**

215 - "Pt(II) and Pt(IV) Amido, Aryloxide and Hydrocarbyl Complexes: Synthesis, Characterization, and Reaction with Dihydrogen and Substrates that Possess C–H Bonds" J. R. Webb, C. Munro-Leighton, A. W. Pierpont, J. T. Gurkin, T. B. Gunnoe, T. R. Cundari, M. Sabat, J. L. Petersen, P. D. Boyle Inorg. Chem. **2011**, 50, 4195-4211. (cover article). **CHE-0701247**

216 - "Selectivity and Mechanism of Hydrogen Atom Transfer By an Isolable Imidoiron(III) Complex;" R. E. Cowley, N. A. Eckert, T. R. Cundari, T. Figg, S. Vaddadi, P. L. Holland J. Am. Chem. Soc. **2011**, 133, 9797 – 9811. **DE-FG02-03ER15387**

217 - "Valine 44 and Valine 45 of Human Glutathione Synthetase are Key for Subunit Stability and Negative Cooperativity;" K. D. Slavens, T. R. Brown, K. A. Barakat, T. R. Cundari, M E. Anderson Biochem. Biophys. Res. Comm. **2011**, 410, 597 – 601. **1R15GM086833-01 (MEA)**

218 - "Non-Redox Oxy-Insertion via Organometallic Baeyer-Villiger Transformations: A Computational Hammett Study of Platinum(II) Complexes;" T. M. Figg, T. R. Cundari, T. B. Gunnoe Organometallics **2011**, 30, 3779 – 3785. **DE-SC0001298**.

219 - "Aspartate 458 of Human Glutathione Synthetase is Important for Cooperativity and Active Site Structure;" T. Brown, M. L. Drummond, S. Barelier, A. Dinescu, S. Hernandez, A. S. Crutchfield, K. D. Slavens, T. R. Cundari, M. E. Anderson Biochem. Biophys. Res. Comm. **2011**, 411, 536 – 542. **1R15GM086833-01 (MEA)**

220 - "A Masked Two-Coordinate Cobalt(I) Complex That Activates C-F Bonds;" T. R. Dugan, X. Sun, O. Olatunji-Ojo, T. R. Cundari, E. V. Rybak-Akimova, P. L. Holland J. Am. Chem. Soc. **2011**, 133, 12418 – 12421 (communication) (7/25/11). **DE-FG02-03ER15387**

221 - "Reaction Mechanism of the Reverse Water-gas Shift Reaction Using First-row Middle Transition Metal Catalysts L'M(M: Fe, Mn, Co): A Computational Study;" C. Liu, T. R. Cundari, A. K. Wilson Inorg. Chem. **2011**, 50, 8782 - 8789. **BER-08ER64603**

222 - "Dinitrogen Activation by Low-Coordinate Transition Metal Complexes;" A. W. Pierpont, T. R. Cundari J. Coord. Chem. **2011**, 64, 3123 – 3135. **CHE-0701247**

223 - "A First-principles Study of Diatomic NiAl: Ground State, Structure, and Spectroscopic Constants;" T. R. Cundari, S. S. Janardan, O. Olatunji-Ojo, B. R. Wilson Intern. J. Quantum Chem. **2011**, 111, 4303 – 4308. **FA8650-08-C-5226**

224 - "DFT Study of the Reactivity of Methane and Dioxygen with d^{10}-L_2M Complexes;" B. M. Prince, T. R. Cundari J. Organomet. Chem. (Caulton Special Issue, "Small Molecule Activation and Catalysis Using Metal-Carbon Multiple Bonds" **2011**, 696, 3982 – 3986 (invited). **DE-SC0001298**

225 - "Mechanistic Studies of Ethylene Hydrophenylation Catalyzed by Bipyridyl Pt(II) Complexes;" B. A. McKeown, H. E. Gonzalez, M. R. Friedfeld, T. B. Gunnoe, T. R. Cundari, M. Sabat J. Am. Chem. Soc. **2011**, 133, 19131 - 19152. **DE-FG02-03ER15387**

226 - "Synthesis and Characterization of $(smif)_2M^n$ (n = 0, M = V, Cr, Mn, Fe, Co, Ni, Ru; n = +1, M = Cr, Mn, Co, Rh, Ir; smif = 1,3-(2-pyridyl)-2-azaallyl);" B. A. Frazier, E. R. Bartholomew, P. T. Wolczanski, S. DeBeer, M. Santiago-Berrios, E. B. Lobkovsky, S. C. Doucette, S. Mossin, K. Meyer, T. R. Cundari – Inorg. Chem. **2011**, 50, 12414 – 12436. **DE-FG02-03ER15387**

227 - "DFT Study of Group 8 Catalysts for the Hydroarylation of Olefins: Influence of Ancillary Ligands and Metal Identity;" T. R. Cundari, G. R. Morello J. Organomet. Chem. **2012**, 697, 15 - 22. **DE-FG02-03ER15387**

228 - "Thermal Conduction Analysis of Layered Functionally Graded Materials;" O. A. Olatunji-Ojo, S. K. S. Boetcher, T. R. Cundari Comp. Mat. Sci. **2012**, 54, 329 – 335. **FA8650-08-C-5226**

229 - "A Computational Comparison of Ni^{II} and Pt^{II} Hydrido-tris(pyrazolyl)borate Supported Hydroarylation Catalysis;" T. R. Cundari, H. E. Gonzalez J. Mol. Cat. A **2012**, 353 – 354, 1 - 6. (Editor's Choice Article). **DE-FG02-03ER15387**

230 - "DFT Modeling of a Methane-to-Methanol Catalytic Cycle via Group 6 Organometallics. The Role of Metal in Determining the Mode of C—H Activation;" K. M. Carsch, T. R. Cundari Comp. Theo. Chem. **2012**, 980, 133 – 137. **DE-SC0001298**

231 - DFT Study of Methane C—H Activation by Pt^{II}-N-Heterocyclic Carbene Complexes. The Importance of Having the Ligands in the Right Place at the Right Time;" B. P. Prince, T. R. Cundari Organometallics **2012**, 31, 1042 – 1048. **DE-SC0001298**

232 - "Metal Mediated Carbon-Oxygen Bond Formation via Organometallic Baeyer-Villiger Transformations: A Computational Study on the Impact of Metal Identity;" T. M. Figg, J. R. Webb, T. R. Cundari, T. B. Gunnoe J. Am. Chem. Soc. **2012**, 134, 2332 – 2339. **DE-SC0001298**

233 - CO_2 Reduction on Transition Metal (Fe, Co, Ni, and Cu) Surfaces: In Comparison with Homogeneous Catalysis;" C. Liu, T. R. Cundari, A. K. Wilson J. Phys. Chem. C **2012**, 116, 5681 – 5688. **BER-08ER64603**

234 - "Carbon Dioxide Migration Pathways in Proteins;" M. L. Drummond, A. K. Wilson, T. R. Cundari J. Phys. Chem. Lett. **2012**, 3, 830 - 833. **BER-08ER64603**

235 – "Coordination Chemistry of 4-methyl-2,6,7-trioxa-1-phosphabicyclo[2,2,1]heptane: Preparation and Characterization of Ru(II) Complexes;" E. E. Joslin, T. B. Gunnoe, M. Sabat, C. L. McMullin, T. R. Cundari, W. H. Myers Inorg. Chem. **2012**, 51, 4791 – 4801. **DE-FG02-03ER15387**

236 - "Surface Interactions of an Au(I) Cyclo-trimer with Au(111) and Al(111) Metal Slabs: A Computational Study;" B. Chilukuri, T. R. Cundari Surface Science **2012**, 606, 1100 - 1107. **CHE-0911690**

237 - "The Importance of Secondary Structure Interactions in CO_2-Protein Binding Patterns;" T. R. Cundari, M. L. Drummond, A. K. Wilson J. Mol. Mod. **2012**, 18, 2527 - 2541. **BER-08ER64603**

238 - "Bifunctional Reactivity of a Nickel-Imide in C-H Functionalization;" S. Wiese, J. McAfee, D. R. Pahls, C. L. McMullin, T. R. Cundari, T. H. Warren J. Am. Chem. Soc. **2012**, 134, 10114 – 10121. **DE-FG02-03ER15387**

239 - "The Role of Iron-β-diketiminate Fragments and Potassium Promoters in N_2 Fixation;" T. M. Figg, P. L. Holland, T. R. Cundari Inorg. Chem. **2012**, 51, 7546 - 7550. **CHE-1057785 and CHE-0701247. Featured in Virtual Issue on Models of Metalloenzymes: http://pubs.acs.org/page/vi/2013/models-of-metalloenzymes.html**

240 - "A Mechanistic Study of Oxy-insertion into Nickel-Carbon Bonds with Nitrous Oxide;" T. M. Figg, T. R. Cundari Organometallics **2012**, 31, 4998 - 5004. **DE-SC0001298**

241 – "Synthetic Approaches to $(smif)_2Ti$ (smif = 1,3-di-(2-pyridyl)-2-azaallyl) Reveal Redox Non-Innocence and C-C Bond-Formation;" B. A. Frazier, P. T. Wolczanski, I. Keresztes, S. DeBeer, E. B. Lobkovsky, A. W. Pierpont, T. R. Cundari Inorg. Chem. **2012**, *51*, 8177–8186. **CHE-1057785**

242 - "Flavin-catalyzed Insertion into Rhenium-Methyl Bonds;" M. J. Pouy, E. M. Milczek, T. B. Gunnoe, T. M. Figg, B. M. Prince, B. M. Otten, T. R. Cundari, J. T. Groves J. Am. Chem. Soc. **2012**, 134, 12920 - 12923. **DE-SC0001298**

243 - "Protein-Based Carbon Capture: Progress and Potential;" M. L. Drummond, T. R. Cundari, A. K. Wilson Greenhouse Gas. Sci. Tech. **2012**, *2*, 223 - 228. (Perspective). (invited). **BER-08ER64603**

244 - "Intramolecular Hydroalkoxylation and Hydroamination of Alkynes Catalyzed by Cu(I) Complexes;" S. A. Delp, J. Uddin, N. A. Cochrane, T. B. Gunnoe, T. R. Cundari, M. Sabat ACS Catalysis **2012**, 2, 2182 - 2193. **CHE-1057785 and CHE-0701247**

245 – "Reductive Elimination of Alkylamines from Low-Valent Palladium (II) Alkyl-Amido Complexes;" P. S. Hanley, S. L. Marquard, T. R. Cundari, J. F. Hartwig J. Am. Chem. Soc. **2012**, 134, 15281–15284 (communication). **CENTC**

246 – "Catalytic Hydroarylation of Olefins Using TpRu(L)(NCMe)Ph (L = 2,6,7-Trioxa-1-phosphabicyclo[2,2,1]heptane): Comparison to TpRu(L')(NCMe)Ph Systems [L' = CO, PMe_3, $P(pyr)_3$ or $P(OCH_2)_3CEt$)];" E. E. Joslin, T. B. Gunnoe, M. Sabat, C. L. McMullin, T. R. Cundari, W. H. Myers – Organometallics **2012**, 31, 6851 - 6860. **DE-FG02-03ER15387**

247 - "The Nature of Protein-CO_2 Interactions as Elucidated via Molecular Dynamics," M. L. Drummond, A. K. Wilson, and T. R. Cundari, J. Phys. Chem. B **2012**, 116, 11578 - 11593. **BER-08ER64603**

248 - "An ab initio study on interaction energies of CO_2-amine complexes: Effects of amine substituents;" K. R. Jorgensen, T. R. Cundari, A. K. Wilson J. Phys. Chem. B 2012, 116, 10403 - 10411. **BER-08ER64603**

249 – "Reaction of Cu^I with Dialkylperoxides: Cu^{II}-alkoxides, Alkoxy Radicals and C-H Etherification;" R. T. Gephart III, C. L. McMullin, N. Sapiezynski, E. S. Jang, M. J. B. Aguila, T. R. Cundari, T. H. Warren J. Am. Chem. Soc. **2012**, 134, 17350 – 17353. (communication). **CHE-1057785**

250 - "Unusual Biomimetic Pathway for Intramolecular Vanadium(V)- Aerobic Oxidation: Evidence for Base-assisted Oxidation of Benzyl Alcoholate Ligand;" B. N. Wigington, S. K Hanson, M. L. Drummond, T. R. Cundari, D. L. Thorn, S. L. Scott Chem. Eur. J. **2012**, 19, 14981 – 14988. **CENTC**

251 - "Single-Electron Oxidation of N-Heterocyclic Carbene-Supported Nickel Amides Yielding Benzylic C-H Activation;" C. A. Laskowski, G. R. Morello, C. T. Saouma, T. R. Cundari, G. L. Hillhouse Chem. Sci. (Edge Article) **2013**, 4, 170 - 174. **DE-FG02-03ER15387**

252 - "Variable Pathways for Oxygen Atom Insertion into Metal–Carbon Bonds: The Case of $Cp^*W(O)_2(CH_2SiMe_3)$;" J. J. Mei, K. M. Carsch, C. R. Freitag, T. B. Gunnoe, T. R. Cundari J. Am. Chem. Soc. **2013**, 135, 424 – 435. **DE-SC0001298**

253 - "Mechanism of Hydrogenolysis of an Iridium-Methyl Bond: Evidence for a Methane Complex Intermediate;" J. Campos, E. Carmona, M. Brookhart, S. Kundu, D. R. Pahls, T. R. Cundari J. Am. Chem. Soc. **2013**, 135, 1217 – 1220 (communication). **CENTC**

254 - "Metal Mediated Oxo Insertion into Platinum-Carbon Bonds: A Computational Hammett Analysis;" T. M. Figg, T. R. Cundari Dalton Trans. (Mechanistic Organometallic Chemistry special issue; Crabtree, R. H., Ed.) **2013**, 42, 4114 - 4121 (invited). **DE-SC0001298**

255 - "Periodic Trends in Metal Mediated CO_2 Activation;" C. Liu, T. R. Cundari, A. K. Wilson in "Applications of Molecular Modeling to Challenges in Clean Energy;" American Chemical Society Symposium Series, G. Fitzgerald, N. Govind (Eds.), ACS: Washington, D. C., **2013**, Chapter 5, pp. 67 – 88. **BER-08ER64603**

256 - "Complete Methane-to-Methanol Catalytic Cycle: A DFT Study of Oxygen Atom Transfer from N_2O to late-row (M = Ni, Cu, Zn) β-diketiminate C—H Activation Catalysts;" C. M. McMullin, A. W. Pierpont, T. R. Cundari Polyhedron **2013** 52, 945 - 956. (invited, Special Issue, 100th Anniversry of the Award of the 1913 Nobel Prize in Chemistry to Alfred Werner). **DE-SC0001298**

257 - "Selective Extraction of N_2 from Air by Diarylimine Iron Complexes;" E. R. Bartholomew, E. C. Volpe, P. T. Wolczanski, E. B. Lobkovsky, T. R. Cundari J. Am. Chem. Soc. **2013**, 135, 3511 - 3527. **DE-FG02-03ER15387**

258 - "C-C Bond Formation and Related Reactions at the CNC Backbone in (smif)FeX (smif = 1,3-di-(2-pyridyl)-2-azaallyl): Dimerizations, 3+2 Cyclization, and Nucleophilic Attack; Hydrogenations and Alkyne Trimerization (X = $N(TMS)_2$, dpma (di-(2-pyridyl-methyl)-amide));" B. A. Frazier, P. T. Wolczanski, S. C. Bart, K. Meyer, T. R. Cundari, E. B. Lobkovsky Inorg. Chem. **2013**, 52, 3295 - 3312. **CHE-1057785**

259 - "Facile and Regioselective C–H Bond Activation of Aromatic Substrates by an Fe(II) Complex Involving a Spin-Forbidden Pathway;" S. E. Kalman, A. Petit, T. B. Gunnoe, D. H. Ess, T. R. Cundari, M. Sabat Organometallics **2013**, 32, 1797 - 1806. **DE-FG02-03ER15387**

260 - "Pt(II) Catalyzed Ethylene Hydrophenylation: Switching Selectivity between Alkyl and Vinyl Benzene Production;" B. A. McKeown, H. E. Gonzalez, M. R. Friedfeld, A. M. Brosnahan, T. B. Gunnoe, T. R. Cundari, M. Sabat Organometallics **2103**, 32, 2857 - 2865. **DE-FG02-03ER15387**

261 - "Use of $[SbF_6]^-$ to Isolate Cationic Copper and Silver Adducts with More than one Ethylene on the Metal Center;" M. Fianchini, C. F. Campana, B. Chilukuri, T. R. Cundari, V. Petricek, H. V. R. Dias Organometallics **2013**, 32, 3034 – 3041. **CHE-1057785 and CHE-0701247**

262 - "Pt^{II} Catalyzed Ethylene Hydrophenylation: Influence of Dipyridyl Chelate Ring Size on Catalyst Activity and Longevity;" B. A. McKeown, H. E. Gonzalez, T. B. Gunnoe, T. R. Cundari, M. Sabat ACS Catalysis **2013**, 3, 1165 - 1171. **DE-FG02-03ER15387**

263 - "Electronic Properties in Trinuclear Gold Crystals: Equivalent Three-dimensional Electron Transport and Remarkable One-dimensional Hole Transport;" L. Zhu, B. Chilukuri, V. Coropceanu, J-L. Bredas, T. R. Cundari J. Phys. Chem. Lett. **2013**, 4, 21856 - 2189. **CHE-0911690**

264 - "Control of Olefin Hydroarylation Catalysis via a Sterically and Electronically Flexible Pt(II) Catalyst Scaffold;" B. A. McKeown, H. E. Gonzalez, T. Michaelos, T. B. Gunnoe, T. R. Cundari, R. H. Crabtree, M. Sabat Organometallics **2013**, 32, 3903 – 3913. **DE-FG02-03ER15387**

265 – "C-H Activation by Multiply Bonded Complexes with Potentially Non-Innocent Ligands: A Computational Study;" O. A. Olatunji-Ojo, T. R. Cundari Inorg. Chem. **2013**, 52, 8106 - 8113. **CHE-1057785**

266 - "Cooperative Carbon Capture Capabilities in Multivariate MOFs Decorated with Amino Acid Side Chains: A Computational Study; M. L. Drummond, T. R. Cundari, A. K. Wilson J. Phys. Chem. C. **2013**, 117, 14717 - 14722. **BER-08ER64603**

267 - "Computational Study of Carbon-Hydrogen Bond Activation by Alkali Metal Superbases;" D. B. Pardue, S. J. Gustafson, D. H. Ess, T. R. Cundari Comp. Theo. Chem. **2013**, 1019, 85 - 93. **DE-SC0001298**

268 - "Lewis Bases Trigger Intramolecular CH-Bond Activation: $(silox)_2W{=}N^tBu$ <=> $(silox)(\kappa^2\text{-}O,C\text{-}OSi^tBu_2CMe_2CH_2)HW{=}N^tBu$ (silox = OSi^tBu_3);" M. Marshak, D. C. Rosenfeld, W.D. Morris, P. T. Wolczanski, E. B. Lobkovsky, T. R. Cundari Eur. J. Inorg. Chem. **2013**, 4056 - 4067. (invited) **DE-FG02-03ER15387**

269 - "Pt(II) and Rh(III) Hydrocarbyl Complexes Bearing Coordinated Oxygen Atom Delivery Reagents;" J. R. Webb, T. M. Figg, B. M. Otten, T. B. Gunnoe, T. R. Cundari, M. Sabat Eur. J. Inorg. Chem. **2013**, 4515 - 4525. **DE-SC0001298**

270 – "Spin Crossover during β-hydride Elimination in High-spin Iron(II) and Cobalt(II) Alkyl Complexes;" S. M. Bellows, T. R. Cundari, P. L. Holland Organometallics **2013**, 32, 4741 – 4851. **DE-FG02-03ER15387**

271 - "Palladium Oxo Complexes as Intermediates in Metal-Carbon Bond Oxy-Insertion. Analysis of their Bonding and Structure by Density Functional and Correlated Wavefunction Methods;" T. M. Figg, G. Schoendorff, B. Chiulukuri, T. R. Cundari Organometallics **2013**, 32, 4993 - 4996. **DE-SC0001298**

272 – "Chemical Bonds Involving d-Orbitals;" invited Viewpoint Chem. Comm. **2013**, 49, 9521 - 9525.

273 - "Methane C—H Bond Activation by "Naked" Alkali Metal Imidyl and Alkaline Earth Metal Imide Complexes. The Role of Ligand Spin and Nucleophilicity;" B. M. Prince, T. R. Cundari J. Phys. Chem. A **2013**, 117, 9245 - 9251. **DE-FG02-03ER15387**

274 – "Silver(I) complexes of tris(pyrazolyl)borate ligands bearing six trifluoromethyl and three additional electron-withdrawing substituents;" N. B. Jayaratna, D. B. Pardue, M. Yousufuddin, K. G. Thakur, T. R. Cundari, H. V. R. Dias Dalton Trans. **2013**, 42, 15399 - 15410. **CHE-1057785**

275 – "Gold mediated expulsion of dinitrogen from organic azides;" C. Dash, M. Yousufuddin, T. R. Cundari, H. V. R. Dias J. Am. Chem. Soc. **2013**, 135, 15479 – 15488. **DE-FG02-03ER15387**

276 - "Activation of Carbon–Hydrogen Bonds by 1,2-CH-addition Across Metal–Heteroatom Bonds;" J. R. Webb, S. A. Burgess, T. R. Cundari, T. B. Gunnoe Dalton Trans. **2013**, 42, 16646 - 16665. (Perspective). (invited). **DE-FG02-03ER15387**

277 - "DFT Study of Oxygen Atom Insertion into Metal–Methyl Bonds of Fe(II), Ru(II) and Os(II) Complexes: Study of Metal-Mediated C–O Bond Formation;" D. B. Pardue, J. J. Mei, T. B. Gunnoe, T. R. Cundari Inorg. Chem. **2014**, 53, 2968 – 2975. **DE-SC0001298**

278 - "Oxy-functionalization of Group 9 and 10 Transition Metal Methyl Ligands: Use of Pyridine-based Hemi-labile Ligands;" B. M. Prince, T. B. Gunnoe, T. R. Cundari Dalton Trans. **2014**, 43, 7608 – 7614. **DE-SC0001298**

279 - "Theoretical Study of Reductive Functionalization of Methyl Ligands of Group 9 Complexes Supported by Two Bipyridyl Ligands: A Key Step in Catalytic Hydrocarbon Functionalization;" D. R. Pahls, J. T. Groves, T. B. Gunnoe, T. R. Cundari Organometallics **2014**, 33, 1936 - 1944. **DE-SC0001298**

280 – "Reductive Functionalization of a Rh(III)-methyl Bond by Electronic Modification of the Supporting Ligand;" M. E. O'Reilly, D. R. Pahls, J. R. Webb, N. C. Boaz, S. Majumdar, C. D. Hoff, J. T. Groves, Thomas R. Cundari, T. B. Gunnoe Dalton Trans **2014**, 43, 8273 - 8281. **DE-SC0001298**

281 - "C–H Activation of Pyrazolyl Ligands by Ru(II);" E. E. Joslin, B. Quillian, T. B. Gunnoe, T. R. Cundari, M. Sabat, W. H. Myers Inorg. Chem. **2014**, 53, 6270 - 6278. **DE-FG02-03ER15387**

282 – "Iron Complexes Derived from {nacnac-$(CH_2py)_2$}$^-$ and {nacnac-$(CH_2py)(CHpy)$}^{n} Ligands: Stabilization of Fe(II) via Redox Non-innocence;" V. A. Williams, P. T. Wolczanski, J. Sutter, K. Meyer, E. B. Lobkovsky, T. R. Cundari Inorg. Chem. **2014**, 53, 4459 - 4474. ***CHE-1057785***

283 - "Pt^{II} Catalyzed Hydrophenylation of α-Olefins: Variation of Linear: Branched Products as a Function of Ligand Donor Ability;" B. A. McKeown, B. M. Prince, Z. Ramiro, T. B. Gunnoe, T. R. Cundari ACS Catalysis **2014**, 4, 1607 - 1615. **DE-FG02-03ER15387**

284 - "Impact of d-Orbital Occupation on Metal Carbon Bond Functionalization;" E. C. Garrett, T. M. Figg, T. R. Cundari Inorg. Chem. **2014**, 53, 7789 – 7798. **DE-SC0001298**

285 - "Molecular and Electronic Structure of Cyclic Trinuclear Au(I) Carbeniate Complexes. Insight for Structure/Luminescence/Conductivity Relationships;" R. N. McDouglad Jr., B. Chilukuri, H. Rabaâ, O. Elbjeirami, X. Wang, V. Nesterov, T. R. Cundari, M. A. Omary Inorg. Chem. **2014**, 53, 7485 -7499. **CHE-0911690**

286 - "Iron and Chromium Complexes Containing Tridentate Chelates Based on Nacnac and Imino- and Methyl-Pyridine Components: Triggering C-C(X) Bond Formation;" W. D. Morris, P. T. Wolczanski, J. Sutter, K. Meyer, T. R. Cundari, E. B. Lobkovsky Inorg. Chem. **2014**, 53, 7467 – 7484. **CHE-1057785**

287 - "Modeling of Late 3d Transition Metal Metathesis of tert-Butoxide Complexes with Amines;" F. Birk, C. R. Freitag, T. R. Cundari, W. Ou, T. R. Cundari Polyhedron **2014**, 80, 112 - 116. **DE-FG02-03ER15387**

288 - "Copper(II) Anilides in sp^3 C-H Amination;" Jang, E.; McMullin, C. L.; Kaβ, M.; Meyer, K.; Cundari, T. R.; Warren, T. H. J. Am. Chem. Soc. **2014**, 136, 10930 – 10940. **CHE-1057785**

289 - "Iridium, Rhodium and Ruthenium Catalysts for the "Aldehyde-Water Shift" Reaction;" T. P. Brewster, W. C. Ou, J. C. Tran, K. I. Goldberg, S. K. Hanson, T. R. Cundari, D. M. Heinekey ACS Catalysis **2014**, 4, 3034 – 3038. (letter). **CENTC**

290 - "A Versatile Tripodal Cu(I) Reagent for C–N Bond Construction via Nitrene-Transfer Chemistry: Catalytic and Mechanistic Perspectives on C–H Aminations/Amidinations and Olefin Aziridinations;" V. Bagchi, P. Paraskevopoulou, P. Das, L. Chi, Q. Wang, A. Choudhuri, J. Mathieson, L. Cronin, D. B. Pardue, T. R. Cundari, Y. Sanakis, P. Stavropoulos J. Am. Chem. Soc. **2014**, 136, 11362 – 11381. **CHE-1057785**

291 - "The Role of Strong Electrostatic Interactions at the Dimer Interface of Human Glutathione Synthetase;" M. De Jesus, B. L. Ingle, T. R. Cundari, M. E. Anderson Protein Journal **2014**, 33, 403 – 409. **1R15GM086833-01 (MEA)**

292 - "Hydrophenylation of Ethylene using a Cationic Ru(II) Catalyst: Comparison to a Neutral Ru(II) Catalyst;" S. A. Burgess, E. E. Joslin, T. B. Gunnoe,T. R. Cundari, M. Sabat, W. H. Myers Chem. Sci. (Edge Article) **2014**, 5, 4355 – 4366. **DE-FG02-03ER15387**

293 - "Oxygen Atom Insertion into Iron Phenyl and Methyl Bonds to Produce Phenol and Methanol: A Key Step for Catalytic Hydrocarbon Functionalization;" J. J. Mei, S. E. Kalman, D. B. Pardue, T. B. Gunnoe, T. R. Cundari, M. Sabat Organometallics **2014**, 33, 5597 – 5605. **DE-SC0001298**

294 - "The Curious Case of Mesityl Azide and Its Reactivity with bpyNiEt_2;" T. M. Figg, B. M. Otten, G. L. Hillhouse, T. R. Cundari Inorg. Chem. **2014**, 53, 11633 – 11639. **DE-FG02-03ER15387**

295 - "DFT Study of the Reaction of a Two-Coordinate Iron(II) Dialkyl Complex with Molecular Oxygen;" B. M. Prince, T. R. Cundari, C. J. Tymczak J. Phys. Chem. A **2014**, 118, 11056 – 11061.

296 – "Disparate Reactivity from Isomeric {$Me_2C(CH_2N{=}CHpy)_2$} and {$Me_2C(CH{=}NCH_2py)_2$} Chelates in Iron Complexation;" E. B. Hulley, V. A. Williams, W. D. Morris, P. T. Wolczanski, K. Hernandez-Burgos, E. B. Lobkovsky, T. R. Cundari Polyhedron **2014**, 84, 182 – 191. (invited, Bercaw 70th Birthday Special Issue). **CHE-1057785**

297 – "Impact of Divalent Metal Cations on the Catalysis of Peptide Bonds: A DFT Study;" B. L. Ingle, T. R. Cundari J. Coord. Chem. **2014**, 67, 3920 – 3931. (invited, Costamagna special issue). **CHE-1057785**

298 - "Understanding the Effect of Ancillary Ligand on Concerted Metalation Deprotonation by Phe-box$Ir(OAc)_2(H_2O)$: A DFT Study;" D. R. Pahls, K. E. Allen, K. I. Goldberg, T. R. Cundari Organometallics **2014**, 33, 6413 – 6419. **CENTC**

299 - "Reductive Functionalization of a Rh(III)-methyl Bond in Acidic Media: A Key Step in the Electrophilic Functionalization of Methane;" M. O'Reilly, D. R. Pahls, T. R. Cundari, T. B. Gunnoe Organometallics **2014**, 33, 6504 – 6510. **DE-SC0001298**

300 - "DFT Modeling of the Aldehyde-Water Shift Reaction;" W. C. Ou, T. R. Cundari ACS Catalysis **2015**, 5, 225 – 232. **CENTC**

301 - "Experimental and Computational Studies of the Ruthenium-Catalyzed Hydrosilylation of Alkynes: Mechanistic Insights to Regio- and Stereoselective Formation of Vinylsilanes;" Chae Yi, R. Gao, T. R. Cundari, D. R. Pahls Organometallics **2014**, 33, 6937 – 6944. **DE-FG02- 03ER15387**

302 - "Reactivity Studies of a Three-Coordinate Nickel Complex Featuring a Terminal Imido Ligand. Carbon-Hydrogen Activation, C-N Bond Formation, and Cycloaddition Chemistry;" D. J. Mindiola, R. Waterman, V. M. Iluc, S. Baldwin, T. R. Cundari, G. L. Hillhouse Inorg. Chem. **2014**, 33, 13227 - 13238. **DE-FG02-03ER15387**

303 - "A Comparison of the Simmons-Smith Reaction with Carbenoids to Nitrenoids and Oxenoids;" S. K. Khani, T. R. Cundari Comp. Theor. Chem. **2015**, 1056, 61 - 73. **CHE-1057785**

304 - "A Rhodium Catalyst for Single-Step Styrene Production;" B. A. Vaughan, M. S. Webster-Gardiner, T. R. Cundari, T. B. Gunnoe Science **2015**, 348, 421 – 424. **DE-FG02-03ER15387**

305 - "Oxy Functionalization with $Cp^*Ir^{III}(NHC)(Me)(Cl)$ with O_2: Identification of a Rare Bimetallic Ir^{IV} μ-oxo Intermediate;" M. C. Lehman, D. R. Pahls, J. M. Meredith, R. D. Sommer, D. M. Heinekey, T. R. Cundari, E. A. Ison J. Am. Chem. Soc. **2015**, 127, 3574 – 3584. **CENTC**

306 - Reductive Functionalization of Methyl Ligands by 3d Metal Catalysis;" H. Fallah, T. R. Cundari - Comp. Theor. Chem. **2015**, 1069, 86 - 957/15. **DE-FG02-03ER15387**

307 - "Methane is the Best Substrate for (sp^3)C-H activation with $Cp^*(PMe_3)Co(Me)(OTf)$. A Density Functional Theory Study;" S. M. Bellows, T. R. Cundari, W. D. Jones Organometallics **2015**, 34, 4032 – 4038. **CENTC**

308 - "1st Row Transition Metal and Lithium Pyridine-ene-amide Complexes Exhibiting N- and C-Isomers and Ligand-based Activation of Benzylic C-H Bonds;" B. M. Lindley, P. T. Wolczanski, T. R. Cundari, E. B. Lobkovsky Organometallics **2015**, 34, 4656 – 4668. Hillhouse Memorial Issue. **DE-FG02-03ER15387**

309 - "DFT Study Reductive Functionalization in Cis and Trans Cobalt-Methyl-Bipyridine Complexes. S. L. Teaw, B. W. Thornton, F. Jia, J. Qian, D. R. Pahls, T. R. Cundari Comp. Theor. Chem. **2015**, 1072, 102 – 105. **DE-FG02-03ER15387**

310 - "Effect of Ligand Connectivity and Charge State on the Amination of C–H Bonds by Copper Amide Complexes;" O. Olatunji-Ojo, T. R. Cundari Organometallics **2015**, 34, 5045 – 5-050. **CHE-1057785**

311 – "Nitrene Insertion into CC and CH Bonds of Diamide-diimine Ligated Chromium and Iron Complexes;" S. P. Heins, W. D. Morris, P. T. Wolczanski, E. B. Lobkovsky, T. R. Cundari Angew. Chem., Int. Ed. **2015**, 54, 14407 - 14411. (comm.) **CHE-1057785**

312 - "Zinc(II) Mediated Carbene Insertion into C-H Bonds in Alkanes;" N. Kulkarni, C. Dash, N. Jayaratna, S. Ridlen, S. K. Khani, A. Das, X. Kou, M. Yousufuddin, T. R. Cundari, H. V. R. Dias Inorg. Chem. **2015**, 54, 11043 - 11045. (comm.) **CHE-1057785**

313 – "Gold mediated isomerization of cyclooctyne to ring fused olefinic bicycles;" H. V. R. Dias, A. Das, T. R. Cundari, M. Yousufuddin Eur. J. Inorg. Chem. **2015**, 54, 11043 - 11045 (comm.). **CHE-1057785**

314 - "Transition Metal Mediated C−H Activation and Functionalization: The Role of Poly(pyrazolyl)borate and Poly(pyrazolyl)alkane Ligands;" B. A. McKeown, J. P. Lee, J. Mei, T. R. Cundari, T. B. Gunnoe Euro. J. Inorg. Chem. **2016**, 15 - 16, 2296 – 2311 (invited). **DE-FG02-03ER15387**

315 - "A Density Functional Theory Study of Novel Catalysts for the "Green" Synthesis of Aziridines;" C. S. Guan, T. R. Cundari Comp. Theor. Chem. **2016**, 1091, 64 – 71. **CHE-1464943**

316 - "Iron-Catalyzed Homogeneous Hydrogenation of Alkenes under Mild Conditions by a Stepwise, Bifunctional Mechanism;" R. Xu, S. Chakraborty, S. B. Bellows, H. Yuan, T. R. Cundari, W. D. Jones ACS, Catalysis **2016**, 6, 2127 – 2135. **CENTC**

317 - "Theoretical Study of Two Possible Side Reactions for Reductive Functionalization of 3d Metal-Methyl Complexes by Hydroxide Ion: Deprotonation and Metal-Methyl Bond Dissociation;" Fallah, H.; Horng, F.; Cundari, T. Organometallics **2016**, 35, 950 – 958. **CHE-1464943**

318 - "Reactivity of Hydrogen On and In Nanostructured Molybdenum Nitride: Crotonaldehyde Hydrogenation;" B. Wyvratt, J. Gaudet, D. B. Pardue, A. Marton, S. Rudic, E. A. Mader, T. R. Cundari, J. M. Mayer, L. T. Thompson ACS, Catalysis **2016**, 6, 5797 - 5806. **CENTC**

319 – "A Dinitrogen Dicopper(I) Complex via a Mixed Valence Dicopper Hydride;" Zhang, S.; Fallah, H.; Gardner, E. J.; Bertke, J. A.; Cundari, T. R.; Warren, T. H. Angew. Chem. **2016**, 128, 10081 – 10085. **CHE-1464943**

320 – "Competing Amination and C-H Arylation Pathways in Pd/Xantphos-Catalyzed Transformations of Binaphthyl Triflates: Switchable Routes to Chiral Amines and [5]Helicene Derivatives;" A. A. Ruch, S. Handa, F. Kong, V. A. Nesterov, D. R. Pahls, T. R. Cundari, L. M. Slaughter Org. Biomol. Chem. 2016, 14, 8123 – 8140. **CHE-1057785, CHE-1464943**

321 - "Fe(IV) Alkylidenes Are Actually Fe(II), and a Related Octahedral Fe(II) "Alkylidene" Is a Conjugated Vinyl Complex;" B. P. Jacobs, R. G. Agarwal, P. T. Wolczanski, T. R. Cundari, S. N. MacMillan Polyhedron **2016**, 116, 47 – 56. (invited, M. L. Green issue). **DE-FG02-03ER15387**

322 – "The Mechanism of N-N Double Bond Cleavage by an Iron(II)-Hydride Complex;" The Mechanism of N-N Double Bond Cleavage by an Iron(II)-Hydride Complex J. Am. Chem. Soc. **2016**, 138, 12112 – 12123. **DE-FG02-03ER15387**

323 – "N-Heterocyclic Carbene-Based Nickel and Palladium Complexes: A DFT Comparison of the Mizoroki-Heck Catalytic Cycles;" V. H. M. da Silva, A. Braga, T. R. Cundari Organometallics **2016**, 35, 3170 - 3181. **DE-FG02-03ER15387**

324 – "Density Functional Study of Oxygen-Insertion into Niobium-Phosphorus Bonds: Novel Mechanism for Liberating P_3^- Synthons;" G. R. Morello, T. R. Cundari Organometallics 2016, 35, 3624 - 3634. **DE-FG02-03ER15387**

325 – "Solvent-Dependent Thermochemistry of an Iridium/Ruthenium H_2 Evolution Catalyst;" K. R. Brereton, C. L. Pitman, T. R. Cundari, A. J. M. Miller Inorg, Chem. **2016**, 55, 12042 – 12051. **CENTC**

326 – "Aqueous Hydricities from Calculations of Reduction Potential and Acidity in Water " Brereton, K.; Bellows, S. M.; Fallah, H.; Lopez, A. A.; Adams, R. M.; Miller, A. J.; Jones, W. D.; Cundari, T. R. J. Phys. Chem. B **2016**, 120, 12911 – 12919. **CENTC**

327 - "The Effect of Ancillary Ligands on Oxidative Addition of CH_4 to Ta(III) Complexes: A = B, Al, CH, SiH, N, P;" R. Parveen, T. R. Cundari Organometallics **2017**, 36, 64 – 73. Invited. **CHE-1464943**

328 – "Mechanistic Studies of Single-Step Styrene Production Using a Rhodium(I) Catalyst;" B. A. Vaughan, S. K. Khani, J. B. Gary, J. D. Kammert, M. S. Webster-Gardiner, B. A. McKeown, R. J. Davis, T. R. Cundari, T. B. Gunnoe J. Am. Chem. Soc. **2017**, 139, 1486 - 1498. **DE-FG02-03ER15387**

329 – "5d Metal(IV) Imide Complexes. The Impact (or Lack Thereof) of d-Orbital Occupation on Methane Activation and Functionalization;" C. A. Moulder, T. R. Cundari Inorg. Chem. **2017**, 56, 1823 – 1829. **CHE-1464943**

330 – "DFT Investigation of C-F Bond Activation by a Low Coordinate Cobalt(I) Complex;" Jiang, Q.; Cundari, T. R. Comp. Theo. Chem. **2017**, 1105, 97 - 103. **CHE-1464943**

331 - "An Uncanny Dehydrogenation Mechanism: Polar bond control over stepwise or concerted transition states;" S. M. Bellows, J. B. Gary, S. Chakraborty, W. D. Jones, T. R. Cundari Inorg. Chem. 2017, 56, 5529 – 5524. **CENTC**

332 – "Redox non-innocence permits catalytic nitrene carbonylation by (dadi)Ti=NAd (Ad = adamantyl);" S. P. Heins, P. T. Wolczanski, T. R. Cundari, S. N. MacMillan Chem. Sci. **2017**, 8, 3410 - 3418. **DE-FG02-03ER15387**

333 - *"*Elusive Terminal Copper Arylnitrene Intermediates;" A. Bakhoda, Q. Jiang, J. A. Bertke, T. R. Cundari, T. H. Warren Angew. Chem. Int. Ed. **2017**, 56, 6426 – 6430 (communication). **DE-FG02-03ER15387**

334 – "Towards a More Rational Design of the Direct Synthesis of Aniline: A DFT Study;" Z. H. A. Alsunaidi, T. R. Cundari, A. K. Wilson ACS Omega **2017**, 2, 3214 – 3227. **CHE-1057785**

335 - "Three Coordinate Copper(II) Aryls: Key Intermediates in C-O Bond Formation;" S. Kundu, C. Greene, K. Williams, T. Salvador, J. Bertke, T. R. Cundari, T. H. Warren J. Am. Chem. Soc. **2017**, 139, 9112 - 9115. **CHE-1464943**

336 - "Effect of Ancillary Ligands on Oxidative Addition of CH_4 to Re(III) Complexes: A = B, Al, CH, SiH, N, P Using MP2, CCSD(T) and MCSCF Methods;" R. Parveen, T. R. Cundari J. Phys. Chem. A **2017**, 121, 5341 – 5351. **DE-FG02-03ER15387**.

337 – "Heterolytic H-H and H-B Bond Cleavage Reactions of $\{(IPr)Ni(\mu\text{-}S)\}_{2;}$" F. F. Olechnowicz, G. L. Hillhouse, T. R. Cundari, R. F. Jordan Inorg. Chem. **2017**, 56, 9922 – 9930. **DE-FG02-03ER15387**

338 - "Comparison of Pd^{II} vs Rh^{I}-catalyzed Catalytic Cycle for Single Step Styrene Production;" Y. S. Ceylan, T. R. Cundari Comp. Theor. Chem. **2017**, 1115, 313 – 322. **DE-FG02-03ER15387**

339 - "Rare Examples of Fe(IV) Alkyl-imide Migratory Insertions: Impact of Fe-C Covalency in $(Me_2IPr)Fe(=NAd)R_2$ (R = neoPe, 1-nor);" B. P. Jacobs, P. T. Wolczanski, Q. Jiang, T. R. Cundari, S. N. MacMillan J. Am. Chem. Soc. **2017**, 139, 12145 – 12148. (comm.). **DE-FG02-03ER15387**

339 – "Methane Manifesto: A Theorist's Perspective on Catalytic Light Alkane Functionalization;" Comm. Inorg. Chem. T. R. Cundari **2017**, 37, 219 - 237. (invited)

340 - "Studies of the Decomposition of the Ethylene Hydrophenylation Catalyst TpRu(CO)(NCMe)Ph;" E. E. Joslin, B. A. McKeown, T. R. Cundari, T. B. Gunnoe J. Organomet. Chem. **2017**, 847, 289 - 293. Invited (Gladysz special issue). **DE-FG02-03ER15387**

341 – "Methane C-H Activation via 3d Metal-Methoxide Complexes with Potentially Redox Non-innocent Pincer Ligands: A DFT Study;" A. Najafian; T. R. Cundari Inorg. Chem. **2017**, 56, 12282 – 12290. **CHE-1464943**

342 – "Control of C-H Activation by Mo-Oxo Complexes: pK_a or BDFE?;" A. Nazemi; T. R. Cundari Inorg. Chem. **2017**, 56, 12319 – 12327. **CHE-1464943**

343 "Heterobimetallic Silver-Iron Complexes involving $Fe(CO)_5$ ligands;" G. Wang, Y. S. Ceylan, T. R. Cundari, H. V. R. Dias J. Am. Chem. Soc. **2017**, 139, 14292 - 14301. **DE-FG02-03ER15387**

344 - "Computational Study of Methane C−H Activation by Earth-Abundant Metal-Amide/Aminyl Complexes;" B. M. Prince, T. R. Cundari Organometallics **2017**, **36**, 4987 – 3994. **DE-FG02-03ER15387**

345 - "A DFT Survey of the Effects of d-Electron Count and Metal Identity on the Activation and Functionalization of C-H bonds for Mid to Late Transition Metals;" C. A. Moulder, T. R. Cundari Israel J. Chem. **2017**, 57, 1023 - 1031. (Bergman special issue) (invited). **DE-FG02-03ER15387**

346 – "Hydrophenylation of Ethylene Using a Cationic Ru(II) Catalyst: Change in Selectivity Based on an Auxiliary Ligand;" X. Jia, J. B. Gary, B. A. McKeown, S. Gu,, T. R. Cundari, T. B. Gunnoe - Israel J. Chem. **2017**, 57, 1037 – 1046. (Bergman special issue) (invited). **DE-FG02-03ER15387**

347 - "Cooperative Metal+Ligand Oxidative Addition and Sigma-Bond Metathesis: A DFT Study;" K. G. Lopez, T. R. Cundari, J. B. Gary Organometallics **2018**, 37, 309 – 313. **NSF-REU, DE-FG02-03ER15387**

348 – "Computational Analysis of Potential Transition Metal-Terminal Boride Complexes;" Y. S. Ceylan, T. R. Cundari J. Phys. Chem. A **2017**, 121, 9358 – 9368. **DE-FG02-03ER15387**

349 – "Reductive Elimination of Alkylamines from Phosphine-ligated Alkylpalladium(II) Amido Complexes to Form sp^3 Carbon–Nitrogen Bonds;" D. M. Peacock, Q. Jiang, P. S. Hanley, T. R. Cundari, J. F. Hartwig J. Am. Chem. Soc. **2018**, 140, 5893 – 4904. **CENTC**

350 - "DFT Study of Substituent Effects in the Hydroxylation of Methane and Toluene Mediated by an Ethylbenzene Dehydrogenase Active Site Model;" J. O. C. Jimenez-Halla, A. Nazemi, T. R. Cundari J. Organomet. Chem. (special issue "Modern Computational Organometallic Chemistry") **2018**, 864, 44 - 49. **ACS-PRF # 57250-ND6**

351 - "Dispersion Forces Play a Role in $(Me_2IPr)Fe(=NAd)R_2$ (Ad = adamantyl; R = neoPe, 1-nor) Insertions and BDEs;" T. R. Cundari, B. P. Jacobs, S. N. MacMillan, P. T. Wolczanski J. Chem. Soc., Dalton **2018**, 47, 6025 – 6030. (invited, special Power issue). **DE-FG02-03ER15387**

352 - "Computational Study of Methane C–H Activation by Diiminopyridine Nitride Complexes;" Z. Sun, O. A. Hull, T. R. Cundari Inorg. Chem. **2018**, 57, 6807 – 6815. **DE-FG02-03ER15387**

353 - "Computational Study of Acetylene Hydration by Bio-inspired Group Six Catalyst Models;" A. Najafian, T. R. Cundari Polyhedron **2018**, 154, 114 – 122. **ACS-PRF # 57250-ND6**

354 - "Comparative Nitrene-Transfer Chemistry to Olefinic Substrates Mediated by a Library of Anionic Mn(II) Triphenylamido-Amine Reagents and M(II) Congeners (M = Fe, Co, Ni) Favoring Aromatic over Aliphatic Alkenes" V. Bagchi, A. Kalra, P. Das, P. Paraskevopoulou, S. Gorla, L. Ai, Q. Wang, S. Mohapatra, A. Choudhury, Z. Sun, T. R. Cundari, P. Stavropoulos ACS Catalysis **2018**, 8, 9183 – 9206. **DE-FG02-03ER15387**

355 - "Computational Study of the Impact of Ancillary Ligands upon a Tungsten (IV) Imide Complex for Catalytic Methane Functionalization;" E. Montoya, T. R. Cundari Comp. Theor. Chem. **2018**, 1142, 9 - 14. **CENTC**, **CHE-1464943**

356 - "C-H Activation of Methane by Nickel-Methoxide Complexes: A DFT study;" A. Najafian, T. R. Cundari Organometallics **2018**, 37, 3111 – 3121. **CHE-1464943**

357 - "Reductive Elimination from Neopentylpalladium(II) Complexes to Form Primary sp3 Carbon–Nitrogen Bonds;" Peacock, D. M.; Jiang, Q.; Cundari, T. R.; Hartwig, J. F. Organometallics **2018**, 37, 3243 – 3247. **CENTC**

358 - "Complexes of [(dadi)Ti(L/X)]m that Reveal Redox Non-innocence, and a Stepwise Carbene Insertion into a Carbon-carbon Bond;" Heins, S. P.; Morris, W. D.; Cundari, T. R.; MacMillan, S. N.; Lobkovsky, E. B.; Livezey, N.; Wolczanski, P. T. Organometallics **2018**, 37, 3488 – 3501. **DE-FG02-03ER15387**

359 - "Synthesis, photophysical properties, and computational analysis of di- and tetra-nuclear alkyne complexes of copper(I) supported by a highly fluorinated pyrazolate;" D. Parasar, R. Almotawa, N. Jayaratna, Y. S. Ceylan, T. R. Cundari, M. A. Omary, H. V. R. Dias. Organometallics **2018**, 37, 4105 - 4118. **DE-FG02-03ER15387**

360 - "H_2 Addition to $(Me_4PCP)Ir(CO)$: Studies of the Isomerization Mechanism;" T. T. Lekich, J. B. Gary, S. M. Bellows, T. R. Cundari, L. M. Guard, D. M. Heinekey J. Chem. Soc., Dalton **2018**, 47, 16119 - 16125. **CENTC**

361 - "Copper Catalyzed sp^3 C-H Amidation: Sterically Driven 1° and 2° C-H Site-Selectivity;" A. Bakhoda, Q. Jiang, Y. M. Badiei, J. A. Bertke, T. R. Cundari, T. H. Warren Angew. Chem. **2019**, 131, 3459 – 3463. **DE-FG02-03ER15387**

362 - "Carbon(sp^3)-Nitrogen Bond Forming Reductive Elimination from Phosphine-ligated Alkylpalladium(II) Amide Complexes: A DFT Study;" Q. Jiang, D. M. Peacock, J. F. Hartwig, T. R. Cundari Tetrahedron (Special Issue for Computational Chemistry in Organic Synthesis) **2019**, 75, 137 – 143. (invited) **CENTC, CHE-1464943**

363 - "Genetic mutations in the S-loop of human glutathione synthetase: Links between substrate binding, active site structure and allostery;" B. L. Ingle, B. Shrestha, M. C. De Jesus, H. M. Conrad-Webb, M. E. Anderson, T. R. Cundari Comp. Struct. Biotech. J. **2019**, 17, 31 – 38. **1R15GM086833-01 (MEA)**

364 - "Direct Anti-Markovnikov Addition of Water to Olefin to Synthesize Primary Alcohols: A Theoretical Study;" Y. S. Ceylan, T. R. Cundari J. Phys. Chem. A **2019**, 123, 958 – 965. **DE-FG02-03ER15387**

365 – "Oxidative Additions to Ti(IV) in $[(dadi)^{4-}]Ti^{IV}(THF)$ Involve Carbon-carbon Bond Formation and Redox Non-innocent Behavior;" Heins, S. P.; Zhang, B.; MacMillan, S. N.; Cundari, T. R.; Wolczanski, P. T. Organometallics **2019**, 38, 1502 – 1515. **DE-FG02-03ER15387**

366 - "Experimental and computational investigation into the oxidation of an iridium hydride by molecular oxygen;" A. M. Wright, D. R. Pahls, T. Warner, J. Z. Williams, J. B. Gary, S. M. M. Knapp, K. E. Allen, C. R. Landis, T. R. Cundari, K. I. Goldberg J. Am. Chem. Soc. **2019**, 141, 10830 - 10843. **CENTC**

367 - "Intramolecular C–H functionalization followed by a $[2_\sigma+2_\pi]$-addition via an Intermediate Nickel Nitridyl Complex;" J. Ghannam, Z. Sun, T. R. Cundari, M. Zeller, A. Lugosan, C. M. Stanek, W-T. Lee Inorg. Chem. **2019**, 58, 7131 – 7135. (comm.). **DE-FG02-03ER15387**

368 - "Asymmetric Ring-Opening of Donor−Acceptor Cyclopropanes with Primary Arylamines Catalyzed by a Chiral Heterobimetallic Catalyst;" H. Wang, W. Luo, Z. Sun, E. H. N. Fernando, V. N. Nesterov, T. R. Cundari ACS Catalysis. **2019**, 9, 8285 - 8293. **DE-FG02-03ER15387**

369 - "Tungsten-Ligand Bond Strengths for 2p Elements including σ- and π-Bond Strength Components, A DFT and ab initio Study;" Moulder, C. A.; Kafle, K.; Cundari, T. R. J. Phys. Chem. A **2019**, 123, 7940 – 7949. **NSF-GRF (to CAM)**

370 - "Effect of Appended S-block Metal Ion Crown Ethers on Redox Properties and Catalytic Activity of Mn-Nitride Schiff Base Complexes: Methane Activation;" A. Najafian, T. R. Cundari Inorg. Chem. **2019**, 58, 12254 - 12263. **ACS-PRF**

371 - "DFT and QSAR Studies of Ethylene Polymerization by Zirconocene Catalysts;" R. Parveen, G. Rodriguez, J. Younker, T.R. Cundari, L. McCollough ACS Cat. **2019**, 9, 9339 - 9349. **EMCC**

372 - "Nitrene Insertion into Aromatic and Benzylic C–H Bonds Catalyzed by Copper Complexes of Fluorinated Bis- and Tris(pyrazolyl)borates;" T. T. Ponduru; Z. Sun; T. R. Cundari, H. V. R. Dias ChemCatChem **2019**, 11, 4966 – 4973. **DE-FG02-03ER15387**

373 - "Computational Mechanistic Study of Electro-Oxidation of Ammonia to N_2 by Homogenous Ruthenium and Iron Complexes;" A. Najafian, T. R. Cundari J. Phys. Chem. A **2019**, 123, 7973 - 7980. **ACS-PRF**

374 - "Computational Analysis of Proton-Coupled Electron Transfer in Hydrotris(triazolyl)borate Mid – Late 3d, 4d–Transition Metals Complexes;" A. Nazemi, T. R. Cundari Organometallics **2019**, 38, 3521 – 3531. **ACS-PRF**

375 - "Importance of Nitrogen-Hydrogen Bond pKa in the Catalytic Coupling of Alkenes and Amines by Amidate Tantalum Complexes: A Computational Study;" A. Nazemi, T. R. Cundari J. Phys. Chem. A **2019**, 123, 8595 – 8606. **CHE-1464943**

376 - "Computational Study of 3d Metals and Their Influence on the Acidity of Methane C-H Bonds;" C. X. Zhou, T. R. Cundari ACS Omega **2019**, 4, 20159 - 20163. **CHE-1464943**

377 - "Revealing a Decisive Role for Secondary Coordination Sphere Nucleophiles on Methane Activation;" M. E. Anderson, B. Braïda, P. C. Hiberty, T. R. Cundari J. Am. Chem. Soc. **2020**, 142, 3125 – 3131. **Welch B-1985-20190330**

378 - "Synthesis, Characterization, DFT Calculations, and Reactivity Study of a Nitrido-Bridged Dimeric Vanadium(IV) Complex;" A. Lugosan, T. R. Cundari, K. Fleming, D. Dickie, M. Zeller, J. Ghannam, W-T. Lee Dalton Trans. **2020**, 49, 1200 – 1206. **CHE-1464943**

379 - "Unrealized Concepts of Masked Alkylidenes in (PNP)FeXY Systems and Alternative Approaches to $L_nX_mFe(IV)=CHR$;" G. M. George, P. T. Wolczanski, S. N. MacMillan, T. R. Cundari Polyhedron **2020**, 181, 114460 (invited, Bercaw special issue). **CHE-1464943**

380 - "Synthesis, Crystal Structures, and DFT Calculations of Tungsten (IV) and Tungsten (VI) Phosphano Polyhydrides;" M. Yousufuddin, C. C. Carter, B. R. Allen, D. V. Bui, D. A. Daley, C. M. Holinej, J. M. Goncalves, S. Lira, D. E. Muniz, A. I. Santiago, N. Sukran, T. R. Cundari Inorg. Chim Acta **2020**, 508, 119638/1-9. **CHE-1464943**

381 - "Computational Assessment of Counterion Effect of Borate Anions on Ethylene Polymerization by Zirconocene and Hafnocene Catalysts;" R. Parveen, G. Rodriguez, J. Younker, T.R. Cundari Organometallics **2020**, 39, 2068 – 2079. **EMCC**.

382 - "Computational Study of Methane C-H Activation by Main Group and Mixed Main Group-Transition Metal Complexes;" C. C. Carter, T. R. Cundari Molecules **2020**, 25, 2794/1-15 (invited, special issue). **Welch B-1985-20190330**

383 - "Computational Determination of pKa(C–H) in 3d Transition Metal-Methyl Complexes;" W. M. Grumbles, T. R. Cundari Organometallics **2020**, 39, 2803 – 2812. **CHE-1464943**

384 – "Metal and Ligand Effects on Coordinated Methane pKa: Direct Correlation with the Activation Barrier;" A. S. Guan, I. X. Liang, C. X. Zhou, T. R. Cundari J. Phys. Chem A. 2020, 124, 7283 – 7289. **CHE-1464943, CHE-1953547**.

385 - "The first family of structural and functional models for the active site of a unique dioxygenase: Acireductone Dioxygenase (ARD);" G. A. Blade, J. L. Jaies, R. Parveen, W. Illustre, D. Saldana, D. A. Ivan, V. M. Lynch, T. R. Cundari, S. A. Toledo J. Inorg. Biochem. **2020**, 212, 111253/1-10. **CHE-1464943**

386 - "Formal Oxo- and Aza-[3+2] Reactions of α-Enaminones and Quinones: A Double Divergent Process and the Functions of Chiral Phosphoric Acid and Molecular Sieves;" W. Luo, Z. Sun, E. H. N. Fernando, V. N. Nesterov, T. R. Cundari, H. Wang Chem. Sci. **2020**, 11, 9386 – 9394. **CHE-1464943**

387 - "Computational investigations of NHC-derived catalysts for the benzoin condensation;" K. M. Melançon, T. R. Cundari Org. Biomol. Chem. **2020**, 18, 7437 - 7447. **CHE-1464943**

388 - "Plasma-modified Vanadium Oxynitride Surfaces: Characterization by In-situ XPS Experiments and DFT Calculations;" A. Osonkie, V. Lee, P. Chukwunenye, T. R. Cundari, J, A. Kelber J. Chem. Phys. **2020**, 153, 144709/1-9.

389 - "Au_3-to-Ag_3 Coordinate-Covalent Bonding and Other Supramolecular Interactions with Covalent Bonding Strength;" Z. Lou, B. Chilukuri, C. Yang, A. Rawashdeh, R. Arvapally, S. Tekarli, X. Wang, T. R. Cundari, M. A. Omary Chem. Sci. **2020**, 11, 11179 - 11188.

390 – "A Density Functional Study of Methane Activation by Frustrated Lewis Pairs with Group 13 Trihalides and Group 15 Pentahalides;" I. Migliaro, T. R. Cundari J. Chem. Info. Mod. **2020**, 60, 4958 – 4966. **Welch B-1985-20190330**

391 - "Cyclic (Alkyl)(amino)carbenes in Organic and Organometallic Methane C–H Activation: a DFT and MCSCF Study;" Z. Sun, T. R. Cundari PCCP **2020**, 22, 24320 – 24329 (invited, special issue). **CHE-1464943**

392 - "Chemical and Electronic Structures of Cobalt Oxynitride Films Deposited by NH_3 vs. N_2 Plasma: Theory vs. Experiment;" A. Oyelade, A. Osonkie, M. Mrozek-McCourt, T. R. Cundari, J. A. Kelber Phys. Chem. Chem. Phys. **2020**, 22, 24640 – 24648. **CHE-1757946 (REU)**

393 - "DFT Calculations Investigate Competing Pathways to Form Dimeric Neopentylpalladium(II) Amido Complexes: The Critical Importance of Dispersion;" Q. Jiang, T. R. Cundari J. Phys. Chem. A 2020, 124, 8798 – 8805. **CENTC, CHE-1464943**

394 – "Rapid H Abstraction by a Pd^{III} Sulfate Dimer for Methane Monofunctionalization;" R. S. Kim, A. Nazemi, T. R. Cundari, Y. Surendranath ACS Catalysis **2020**, 10, 14782 - 14792. **DE-FG02-03ER15387**

395 – "Thermochemistry of Tungsten-3p Elements, Caveat lector?;" C. A. Moulder, K. Kafle, C. X. Zhou, T. R. Cundari J. Phys. Chem. A **2021**, 125, 681 – 690. **NSF-GRF (to CAM)**

396 - "Electrochemical Reduction of N_2 to Ammonia by Vanadium Oxide Thin Films at Neutral pH: Oxophilicity and the NRR Reaction;" A. Ganesan, A. Osonkie, P. Chukwunenye, I. Rashed, T. R. Cundari, F. D'Souza, J. A. Kelber J. Electrochem. Soc. **2021**, 168, 026504/1-4 (comm.). **CHE-1953547**

397 - "Enantioselective C–H Amination Catalyzed by Nickel Iminyl Com-plexes Supported by Anionic Bisoxazoline (BOX) Ligands;" Y. Dong, C. J. Lund, G. J. Porter, R. M. Clarke, T. R. Cundari, T. A. Betley J. Am. Chem. Soc. **2021**, 143, 817 – 829. **DE-FG02-03ER15387**

398 – "Bifunctional Activation of Methane by Bioinspired Transition Metal Complexes. A Simple Methane Protease Model;" M. E. Anderson, M. B. Marks, T. R. Cundari Comp. Theor. Chem. **2021**, 1198, 113180/1-4. **Welch B-1985-20190330**

399 - "Accessing a Dicopper Nitrenoid *via* Oxidation: Synthesis, Electronic Structure and Bond-Forming Reactivity;" A. N. Desnoyer, A. Nicolay, M. S. Ziegler, K. V. Lakshmi, T. R. Cundari, T. D. Tilley J. Am. Chem. Soc. **2021**, 143, 7135 - 7143. **DE-FG02-03ER15387**

400 - "Synthesis, spectroscopy, and crystallography of mononuclear, five-coordinate aluminum complexes that act as cyclic ester polymerization initiators;" A. McCollum, A. Longo, A. Stahl, A. Butler, A. Rheingold, T. R. Cundari, D. Green, K. Brereton, J, Fritsch Polyhedron **2021**, 204, 115233/1-13.

401 – "DFT calculations on the reaction pathway of multiple intramolecular C-H functionalizations by iron, cobalt and nickel organometallic nitridyl complexes to form amine products;" D. C. Alamo, T. R. Cundari Inorg. Chem. **2021**, 60, 12299 – 12308. **CHE-1953547**

402 - "Reversible C-C Bond Formation, Electromers, and ATRP in Redox Non-Innocent Pyridine-Imine Complexes of Iron;" D. Pokhriyal, S. P. Heins, R. J. Sifri, D. L. Gentekos, R. E. Coleman, P. T. Wolczanski, B. Fors, T. R. Cundari, Thomas; K. M. Lancaster, S. M. MacMillan Inorg. Chem. **2021**, 60, 18662 – 18673. **CHE-1953547**

403 - "Is the Electrophilicity of the Metal Nitrene the Sole Predictor of Metal-Mediated Nitrene Transfer to Olefins? Secondary Contributing Factors as Revealed by a Library of High-Spin Co(II) Reagents;" A. Kalra, V. Bagchi, P. Paraskevopoulou, P. Das, L. Ai, Y. Sanakis, G. Raptopoulos, S. Mohapatra, A. Choudhury, Z. Sun, T. R. Cundari, P. Stavropoulos Organometallics **2021**, 40, 1974 – 1996. CHE-1953547

404 - "Crystal Structure and DFT Calculations of Bis(tetrahydridoborato)bis(cyclopentadienyl)zirconium(IV); N. G. Lopez, C, C. Carter, S. Rocha, C. J. Thomas, K. Falcon, J. Robledo, T. R. Cundari, M. Yousufuddin J. Chem. Crystallogr. **2021**, 51, 1 – 6. **Welch B-1985-20190330**

405 – "Olefin Oligomerization by Zirconium Boratabenzene Catalysts;" C. C. Carter, G. Rodriguez, T. R. Cundari J. Organomet. Chem. **2022**, 962, 122268. **EMCC**

406 - "Investigating the non-classical M-H_2 bonding in $OsClH_3(PPh_3)_3$;" C. C. Carter, R. A. Ryan, W. Zhou, T. Udovic, C. Brown, T. B. Wen, T. R. Cundari, M. Yousufuddin J. Alloys Compounds **2022**, 894, 162445. **Welch B-1985-20190330**

407 - "Electro-catalytic reduction of nitrogen to ammonia: The roles of lattice O and N in reduction at vanadium oxynitride surfaces;" A. Osonkie, A. Ganesan, P. Chukwunenye, F. Anwar, K. Balogun, M. Gharee, I. Rashed, T. R. Cundari, F. D'Souza, J. A. Kelber ACS App. Mat. Interf. **2022**, 14, 531 – 54. **CHE-1953547, DMR-2112864**

408 - "Activation of carbon-hydrogen bonds by complexes involving multiply bonded Group 13 elements;" C. C. Carter, T. R. Cundari Polyhedron **2022**, 219, 115797/1-8. **Welch B-1985-20190330**

409 - "Asymmetric Synthesis of Chromans through Bifunctional Enamine-Metal Lewis Acid Catalysis;" Davis, J.; Gharaee, M.; Karunaratne, C. V. ; Cortes Vazquez, Jose ; Haynes, M. ; Luo, W.; Nesterov, V. N.; Cundari, T. R.; Wang, H. Chem. Euro. J. **2022**, 28, e202200224.

410 - "Group 13 Complexes for Methane Activation;" D. Gupta, T. R. Cundari Comp. Theo. Chem. **2022**, 1214, 113788. **Welch B-1985-20190330**

411 – "Copper(III) Metallacyclopentadienes via Zirconocene-Transfer and Reductive Elimination to an Isolable Phenanthrocyclobutadiene;" Bergman, H.; Beattie, D.; Handford, R.; Suslick, B.; Cundari, T. R.; Liu, Y.; Tilley, T. D. J. Am. Chem. Soc. **2022**, 144, 9853 – 9858. **DE-FG02-03ER15387**

412 – "TEMPO Coordination and Reactivity in Group 6; Pseudo-Pentagonal Planar (η^2-TEMPO)2CrX (X = Cl, TEMPO);" A. K. Kayser, Peter T. Wolczanski, T. R. Cundari, M. M. Bollmeyer, K. M. Lancaster, S. N. MacMillan Chem. Comm. **2022**, 58, 9818 – 9821. **CHE-1953547**

413 – "NO Coupling at Copper to cis-Hyponitrite: N_2O Formation via Protonation and H-atom Transfer;" P. Ghosh, M. Stauffer, V. Hosseininasab, S. Kundu, J. Bertke, T. R. Cundari, T. H. Warren J. Am. Chem. Soc. **2022**, 144, 15093 – 15099. **DE-FG02-03ER15387**

414 - "Metal-Ligand-Anion Cooperation in C–H Bond Formation at Platinum(II);" Zeitler, H. E.; Phearman, A. S.; Gau, M. R.; Carroll, P. J.; Cundari, T. R.; Goldberg, K. I. J. Am. Chem. Soc. **2022**, 144, 14446 – 14451. **CHE-1953547**

415 - "Interaction of molecular nitrogen with vanadium oxide in the absence and presence of water vapor at room temperature: Near-ambient pressure XPS;" K. Balogun, P. Chukwunenye, F. Anwar, A. Ganesan, Q. Adesope, D. Willadsen, S. Nemsak, T. R. Cundari, P. S. Bagus, F. D'Souza, J. A. Kelber. J. Chem. Phys. **2022**, 157, 104701. **DMR-2112864**

416 - "Electrocatalytic Selectivity for Nitrogen Reduction vs. Hydrogen Evolution: A Comparison of Vanadium and Cobalt Oxynitrides at Different pH Values;" P. Chukwunenye, A. Ganesan, M. Gharaee, K. Balogun, F. Anwar, Q. Adesope, T. R. Cundari, F. D'Souza, Jeffry A. Kelber J. Mat. Chem. A **2022**, 10, 21401 – 21415. **DMR-2112864, CHE-1953547**

417 – "Mapping the Basicity of Selected 3d and 4d Transition Metal Nitrides. A DFT Study;" W. S. Alharbi, T. R. Cundari Inorg. Chem. **2022**, 61, 19049 – 19057. **CHE-1953547**

418 – "Three component cascade reaction of cyclohexanones, aryl amines and benzoylmethylene malonates: cooperative enamine-Brønsted acid approach to tetrahydroindoles;" J. C. Vazquez, J. Davis, W. S. Alharbi, A. Moore, V. N. Nesterov, T. R. Cundari, H, Wang, W. Luo ACS Omega **2022**, 7, 45341 – 45346.

419 - "Reactivity of 1.1.1-Propellane with $(silox)_3M$ (M = Ti, V, Cr): Structures of $(silox)_3V{=}(^cC_4H_4){=}CH_2$ and $[(silox)_3Cr–(1.1.1\text{-}C_5H_6)^-]_2$;" G.M. George, P. T. Wolczanski, T. R. Cundari, S. N. McMillan Organometallics **2022**, 41, 3356 – 3365**. CHE-1953547**

420 - "Photo-electrocatalytic Conversion of N_2 to NH_3 by Chemically Modified Transition Metal Dichalcogenides, MoS_2, and WS_2;" A. Ganesan, S. Alhowity, A. Z. Alsaleh, M. Guragain, O. Omolere, R. R. Cundari, J. Kelber, F. D'Souza J. Electrochem. Soc. **2023**, 170, 056501. **DMR-2112864**

421 - "Stability and Activity of Titanium Oxynitride Thin Films for the Electrocatalytic Reduction of Molecular Nitrogen to Ammonia at Different pH Values;" P. Chukwunenye, A. Ganesan, M. Gharaee, K. Balogun, Q. Adesope, S. C. Amagbor, T. D. Golden, F. D'Souza, T. R. Cundari, J. A. Kelber JA.. Physical Chemistry Chemical Physics **2023**, 25, 19540 – 19552. **DMR-2112864, CHE-1953547**

422 - "Crystal Structure and DFT Calculations of $Cp_2NbH(SiIMe_2)(SiFMe_2)$: an Asymmetric Bis(silyl) Niobocene Hydride Complex;" S. M. Rodriguez, Y. N. Motta, M. R. Hill, L. M. Oelke, C. C. Carter, T. R. Cundari, M. Yousufuddin Acta Cryst. C **2023**, C79, 158 – 163.

423 - "Vanadium oxide, Vanadium Oxynitride, and Cobalt Oxynitride as Electrocatalysts for the Nitrogen Reduction Reaction: A Review of Recent Developments;" K. Balogun, A. Ganeshan, P. Chukwunenye, M. Gharaee, S. Nemšák, P. S. Bagus, T. R. Cundari, F. D'Souza, J. A. Kelber J. Phys.: Cond. Matter **2023**, 35, 333002. (invited). **DMR-2112864**

424 - "On the Mechanism of Intermolecular Nitrogen-Atom Transfer from a Lattice-Isolated Diruthenium Nitride Intermediate;" M. Cosio, W. S. Alharbi, A. Sur, C-H. Wang, A. Ezazi, A. Najafian, T. R. Cundari, D. C. Powers Faraday Trans. **2023**, 244, 154 – 168. **DE-FG02-03ER15387**

425 - "Benzimidazole-diamide (bida) Pincer Chromium Complexes: Structures and Reactivity;" A. K. Kayser, P. T. Wolczanski, T. R. Cundari, S. N. MacMillan, M. M. Bollmeyer Organometallics **2023**, 62, 15450 – 15464. **CHE-1953547**

426 - "Nitrene transfer from a sterically confined copper nitrenoid;" K. M. Carsch, S. North, T. Khazanov, A. Iliescu, I. DiMucci, P. Vojackova, Petra; S-L. Zheng, T. R. Cundari, Thomas; K. M. Lancaster, T. A. Betley Chem. Sci. **2023**, 14, 10847 – 10860. **DE-FG02-03ER15387**

427 - "Deciphering the Mechanism of Lewis Base Triggered Conversion of Ammonia to Molecular Nitrogen and Methylamine to Cyanide;" C-P. Chen, W. Alharbi, T. R. Cundari, T. W. Hamann, M. R. Smith III J. Am. Chem. Soc. **2023**, 145, 26339 – 26349. **DE-FG02-03ER15387**

428 - "Transition Metal Nitrosyls: Statistics, Charge Estimates via CDVR, and Studies of Tetradentate Chelate Diamides (pddi)M and (pddi)MNO (M = Cr, Fe, Co);" A. A. D'Arpino, T. R. Cundari, P. T. Wolczanski, S. N. MacMillan Organometallics **2023**, 42, 2747 – 2761. **CHE-1953547**

429 - "Niobium Carbide and Tantalum Carbide as Nitrogen Reduction Electrocatalysts: Catalytic Activity, , Carbophilicity, and the Importance of Intermediate Oxidation States;" S. Alhowity, K. Balogun, A. Ganesan, C. J. Lund, O. Omolere, Q. Adesope, P. Chukwunenye, S. C. Amagbor, F. Anwar, M. K. Altafi, F. D'Souza, T. R. Cundari, J. A. Kelber ACS Appl. Mat. Interfaces – in press (12/12/23). **DMR-2112864**

430 - "DFT study of Vanadium Nitride Alkali Metal complexes for Methane Activation: Impact of Electrostatics;" S. A. Teaw, T. R. Cundari Polyhedron – in press (invite, Wolczanski special issue). **CHE-1953547**

427 - "Non-Oxidative Methane Activation by a Zinc-Based Frustrated Lewis Pair;" K. Bledsoe, S. D. Illesinghe, Y. Gao, L. K. Bennett, J. A. Byrd, S. Hall, C. E. Moore, T. R. Cundari, K. M. Clark J. Am. Chem. Soc. – submitted (11/27/22). **DE-FG02-03ER15387**

429 - "Electrocatalytic Dinitrogen Reduction to Ammonia Using Easily Reducible N-Fused Cobalt Porphyrins;" A. Hajiseyedjavadi, A. Ganesan, P. Rathi, S. Kumar, J. A. Kelber, T. R. Cundari, M. Sankar, F. D'Souza Angew. Chem. – submitted (12/21/23).

431 - "3d and 4d Transition Metals Nitride Mediated N-H Bond Activation: Relevance to the Ammonia Decomposition Reaction;" Alharbi, W. S.; Cundari, T. R. Inorg. Chem. – submitted (7/27/23). **CHE-1953547**

430 – "Chemical and electrocatalytic ammonia oxidation by ferrocene;" M. R. Borougeni, C. Greene, J. A. Bertke, T. R. Cundari, T. H. Warren J. Am. Chem. Soc. – under revision. **DE-FG02-03ER15387**

418 - "Automated Exploration of Methane Activation via Main Group Frustrated Lewis Pairs with Density Functional Theory and Machine Learning;" Chem. Sci. I. Migliaro, T. R. Cundari – submitted (9/21/22). **CHE-1953547**

419 - "Thermodynamic and kinetic analysis of N_2 elimination from late 3d transition metal azido complexes;" C. J. Lund, T. R. Cundari Inorg. Chem. – submitted (10/10/23). **CHE-1953547**

420 – "Copper Catalyzed sp^3 C-H α Acetylation;" O. Okoromoba, E. Jang, C. L. McMullin, T. R. Cundari, T. H. Warren Angew. Chem. – submitted (12/31/20). **DE-FG02-03ER15387**

421 - "Photodynamic properties for phosphorescent d^2, d^6 and d^8 organometallic qubit candidates" D. C. Alamo, T. R. Cundari – manuscript in preparation.

424 – "Using Machine Learning to Predict the pKa of Coordinated Methane and Methyl C-H Bonds;" C. X. Zhou, W. M. Grumbles, T. R. Cundari J. Chem. Info. Mod. – revisions submitted (12/23/20). **CHE-1464943; need to add CHE-1953547**

426 - "Analysis of the concerted metalation-deprotonation in earth abundant 3d-transition-metal mediated C-H activations;" W. M. Grumbles, K. Melancon, T. R. Cundari ACS Catalysis – submitted (5/23/22). DE-FG02-03ER15387

428 - "An Investigation of the Role of Hydrogen-Bonding in Secondary Coordination Sphere Methane Activation;" A. S. Guan, T. R. Cundari – manuscript in preparation. **Welch B-1985-20190330**

431 - "DFT and TDDFT study of photo initiated intermolecular C-H activation and functionalization of toluene, ethylbenzene and cumene by iron, cobalt and nickel nitridyl and amidyl complexes;" D. C. Alamo, W. T. Lee, T. R. Cundari Inorg. Chem. – submitted (2/6/23). **CHE-1953547**

425 - "Oxidative Addition of Pentafluoropyridine to Tertiary Phosphines;" Y. Gao, I. Migliaro, L. K. Bennet, N. Nolan-Dillard, N. Carter, C. E. Moore, T. R. Cundari, K. M. Clark Chem. Comm. – submitted (7/27/23). **DE-FG02-03ER1538.**

426 - "Exploring Nitrogen Vacancy Energies in Titanium/Cobalt Nitrides: A Theoretical Investigation;" Physical Chemistry Chemical Physics – submitted (7/5/23). **CHE-1953547**

Invited Lectures and Contributed (in italics) Presentations

1. "Methane Activation by Transition Metal Complexes;" University of Mississippi, Oxford, Jan. 1993.
2. *"Methane Activation by High-Valent Transition Metal Complexes;" ACS 205th National Meeting, Denver, 1993, paper: INOR207.*
3. *"On the Road to Computer-Aided Catalyst Design: Building a Better Methane Activator;" 10th Florida Catalysis Conference, Palm Coast, April 1993.*
4. "Computational Inorganic Chemistry: Approaches to Transition Metal and Lanthanide Catalysts and Advanced Materials," Los Alamos National Laboratories, CST-3 (Inorganic Chemistry) May 1993.
5. "Computational Approaches to the Computer-Aided Design of C-H Activation Catalysts and Advanced Materials;" Sandia National Laboratories, Albuquerque, May 1993.
6. "Will the Cray ever Replace the CAD-4? Current Trends in Computational Lanthanid Chemistry;" American Crystallographic Association 1993 National Meeting, Albuquerque, May 1993.
7. "Bringing the Promise of Computer-Aided Design to the Rest of the Periodic Table;" Edwards AFB, CA, June 1993.
8. *"On the Road to Computer-Aided Catalyst Design: Building a Better Methane Activator;" Gordon Conference on Organometallic Chemistry, Newport, RI, July 1993.*
9. *"Computational Study of Olefin Metathesis by M(=C(H)R)(XR')(OR")$_2$ Catalysts ;" Gordon Conference on Organometallic Chemistry, Newport, RI, July 1993.*
10. "Methane Activation by Low- and High-Valent Complexes;" ACS 206th National Meeting, Chicago, Symposium on Computational Methods in Inorganic Chemistry, August 1993.
11. "Bringing the Promise of Computer-Aided Design to the Rest of the Periodic Table;" Memphis State University (Dept. of Chemistry), TN, Sept. 1993.
12. "Effective Core Potential and Parallel Computing Approaches to the Study of Methane Activation;" Memphis State University (Dept. of Physics), Sept. 1993.
13. "Parallel Supercomputer-Aided Catalyst Design: Pi-Loading and Methane Activation by High- and Low-Valent Complexes;" University of Arizona, Tucson, Sept. 1993.
14. "Effective Core Potential and Parallel Computing Approaches to the Study of Methane Activation;" University of New Orleans, Oct. 1993.
15. "Computational Inorganic Chemistry at Memphis State University;" Arkansas State University, Oct. 1994. Kickoff Speaker for National Chemistry Week.
16. "Computational Inorganic Chemistry at Memphis State University;" Penn State - Erie, Jan. 1994.
17. "Effective Core Potential and Parallel Computing Approaches to the Study of d- and f-Block Chemistry;" Rochester Institute of Technology, Jan. 1994.
18. "Computational Inorganic Chemistry: Approaches to Transition Metal and Lanthanide Catalysts and Advanced Materials," Kodak, Rochester, Jan. 1994.
19. "Computational Inorganic Chemistry at Memphis State University;" University of Central Arkansas, Feb. 1994.

20. "Computational Inorganic Chemistry: Approaches to Transition Metal and Lanthanide Catalysts and Advanced Materials," University of Alabama-Birmingham, Feb. 1994.
21. "Bringing the Promise of Computer-Aided Design to the d- and f-Block Metals;" ACS 207th National Meeting, Symposium on Actinide, Lanthanide and Early Transition Metal Chemistry, San Diego, March, 1994.
22. "Bringing the Promise of Computer-Aided Design to the Rest of the Periodic Table;" Cornell University, Cornell Theory Center, Cornell National Supercomputer Facility, April 1994.
23. "Activation and Elimination of Hydrocarbons by High-Valent Zr Complexes;" Cornell University, Dept. of Chemistry, April 1994.
24. "Parallel Computing and Effective Core Potential Approaches to Catalysis and Advanced Materials;" University of Delaware, April 1994.
25. "Effective Core Potential and Parallel Computing Approaches to the Study of Catalytically Important Reactions;" Canadian Society of Chemists Meeting, Symposium on Computer-Assisted Methods in Physical and Inorganic Chemistry, Winnipeg, MB, May 1994.
26. "Quantum Modeling of Lanthanide Complexes on Parallel Supercomputers;" Scalable High Performance Computing Conference, Knoxville, TN, May 1994.
27. "Modern Approaches to Computational Organometallic Chemistry;." National Science Foundation Workshop on Organometallics, Corpus Christi, TX, May 1994.
28. "Solving Grand Challenge Problems in Chemistry using Scalable Computing;" Cornell Theory Center, Cornell U, Ithaca, July, 1994.
29. "On the Road to Computer-Aided Catalyst Design: Building a Better Methane Activator;" Catalytica and Associates, Mountainview, CA, Aug. 1994.
30. "Quantum Modeling of CVD Processes for Transition Metal-containing Materials;" Los Alamos National Laboratories, Materials Science Laboratory, Aug. 1994.
31. "Effective Core Potential and Parallel Computing Approaches to Computational Inorganic Chemistry;" University of Missouri-St Louis, Sept. 1994.
32. "Effective Core Potential and Parallel Computing Approaches to d- and f-Block Chemistry;" University of Arkansas, Sept. 1994.
33. "Progress and Future Directions in Computer-Aided Design of Inorganic Materials;" University of Memphis, TN, Sept. 1994.
34. "Progress and Future Directions in Computer-Aided Design of Inorganic Materials;" Murray State University, Kentucky, March 1995.
35. "Computational Studies of the Bonding, Structure, and Reactivity of Naked Main Group Ligands;" ACS 209th National Meeting, Symposium on Naked Main Group Elements as Ligands, Anaheim, April 1995.
36. "Quantum Modeling of Chemical Vapor Deposition (CVD) Processes of Transition Metal-Containing Materials;" ACS 209th National Meeting, Symposium on Inorganic/Organometallic Chemistry in Materials Research, Anaheim, April 1995.
37. "On the Road to Computer-Aided Catalyst Design;" University of Alabama, April 1995.
38. "Modern Approaches to Computational Inorganic Chemistry;" U. of Kentucky, April 1995.
39. "On the Road to Computer-Aided Catalyst Design;" University of Florida, April 1995.
40. "Building a Better Methane Activator;" 12th Florida Catalysis Conference, Palm Coast, April 1995.
41. "On the Road to Computer-Aided Catalyst Design;" Univ. of South Carolina, April 1995.
42. "X-ray Diffraction without X-rays: Computational Methods for Organometallic Complexes;" American Crystallographic Association National Meeting, Montreal, July 1995.
43. *"Computer-aided Design of Inorganic Materials;" Small Molecules Indaba, South African Crystallographic Society, IUCr Commission on Small Molecules, Skukuza, South Africa, 1995.*
44. "X-ray Diffraction without X-rays: Modern Computational Inorganic Chemistry;" Small Molecules Indaba, South African Crystallographic Society, IUCr Commission on Small Molecules, Skukuza, South Africa, 1995.
45. "Computational Inorganic Chemistry at the University of Memphis;" Austin Peay State University, Sept. 1995.
46. "On the Road to Computer-Aided Catalyst Design;" New Mexico State University, October 1995.
47. "Modern Approaches to Computational Inorganic Chemistry: Towards Computer-aided Design of Catalysts and Advanced Materials;" Mississippi State, Oct. 1995.
48. "Effective Core Potential and Parallel Computing Approaches to the Study of d- and f-Block Chemistry;" University of Calgary, November 1995.
49. "Computational Studies of Multiply Bonded Chalcogen and Pnictogen Complexes;" Pac-Basin Chemical Congress, December 1995.

50. "Computational Inorganic Chemistry: Approaches to Transition Metal and Lanthanide Catalysts and Advanced Materials," Auburn, Feb. 1996.
51. "Computational Inorganic Chemistry: Approaches to Transition Metal and Lanthanide Catalysts and Advanced Materials;" Indiana University, Inorganic Chemistry Colloquium, April 1996.
52. "Towards Computer-aided Design of Metal-containing Drugs;" Indiana University, Physical Chemistry Colloquium, April 1996.
53. "Modern Computational Approaches to Organometallic Chemistry;" Gordon Conference on Organometallic Chemistry, Salve Regina U., Newport, R. I., June 1996.
54. "Towards Computer-aided Design of Metal-containing Drugs;" ACS 212th National Meeting, Symposium on Computational Advances in Inorganic Chemistry, Orlando, August 1996.
55. "Computational Inorganic Chemistry: Approaches to Transition Metal and Lanthanide Catalysts and Advanced Materials;" University of Iowa, Oct. 1996.
56. "Computational Studies of Transition Metal Multiply Bonded Complexes: Bonding and Reactivity;" Columbia University, Feb. 1996.
57. "Quantum and Non-quantum Modeling of Inorganic Systems;" 37th Sanibel Symposium, March 1997.
58. "Can Computational Chemistry Tell Us Anything About Building Better CVD Precursors?;" Schumacher Symposium, San Diego, March 1997.
59. "Approaches to Computer-Aided Design of f-Element Complexes;" 3rd Canadian Conference on Computational Chemistry, Edmonton, July 1997.
60. "Modeling Intermolecular Interactions in Inorganic Chemistry;" Small Molecules Indaba II, South African Crystallographic Society, IUCr Commission on Small Molecules, Skukuza, South Africa, August 1997.
61. "Towards the Rational Design of Lanthanide Materials;" South Florida ACS Section, September 1997.
62. "Towards Computer-aided Design of Lanthanide Complexes;" 5th North American Chemical Congress, Cancun, Mexico, Nov. 1997.
63. "Computational Approaches to Modeling Metal-containing Catalysts," Union Carbide, South Charleston, WV, April 1998.
64. "Computational Inorganic Chemistry: Approaches to Transition Metal and Lanthanide Catalysts and Advanced Materials," University of North Carolina-Charlotte, April 1998.
65. "Modeling Transition Metal Catalysts and Advanced Materials," University of South Alabama, Mobile, May 1998.
66. "Modeling C-H Activating Complexes;" Department of Energy, Basic Energy Science Conference, Baltimore, June 1998.
67. "Modeling Transition Metal Catalysts;" Tennessee Technological University, Cookeville, September 1998.
68. "Modeling Transition Metal Catalysts;" University of Texas at Dallas, Richardson, September 1998.
69. "Modeling Transition Metal Catalysts and Advanced Materials," Clark Atlanta University, September 1998.
70. "Modern Approaches to Computational Inorganic Chemistry: Towards Computer-aided Design of Catalysts and Advanced Materials;" University of Bristol (UK), Nov. 1998.
71. "Nontraditional Approaches to Modeling Inorganic Chemistry. Artificial Intelligence and Database Mining;" Univ. Arkansas - Little Rock, Feb. 1999.
72. "Nontraditional Approaches to Modeling Inorganic Chemistry. Artificial Intelligence and Database Mining;" Virginia Commonwealth Univ., Richmond, April 1999.
73. "Nontraditional Approaches to Modeling Inorganic Chemistry. Artificial Intelligence and Database Mining;" Univ. of Cincinnati, Richmond, May 1999.
74. "Time for a New Hammer? Nontraditional Modeling Approaches in Inorganic Chemistry;" National Science Foundation Workshop on Inorganic Chemistry, Belmont, Maryland, June 1999.
75. "Molecular and Semiempirical Modeling of Technetium Chemistry;" Southeast Regional Meeting of the ACS, Symposium on Chemical Recognition Phenomena in Separations, Knoxville, TN, October 1999.
76. "Computational Organometallic Chemistry, Traditional and Nontraditional Modeling Techniques;" Southeast Regional Meeting of the ACS, Symposium on Organometallic and Materials Chemistry in the Southeast, Knoxville, TN, October 1999.
77. "Modeling of Transition Metals with Methods Quantum, Classical and Otherwise;" UNC-Wilmington, April 14, 2000.
78. "Modeling Transition Metal Catalysts and Advanced Materials;" North Carolina State University, April 17, 2000.
79. "Genetic Algorithms for Development of Transition Metal Force Fields;" 220th ACS National Meeting, Washington, D. C., August 2000.

80. "DFT/ECP study of NO scission by M(OR)3 (M = V, Nb, Ta);" 220th ACS National Meeting, Washington, D. C., August 2000.
81. "Application of Modern Computational Methods to Inorganic and Organometallic Chemistry;" University of Tennessee - Knoxville, March 15, 2001.
82. "Application of Modern Computational Methods to Inorganic and Organometallic Chemistry;" Northern Illinois University, April 30,2001
83. "Application of Modern Computational Methods to Inorganic and Organometallic Chemistry;" U of Rochester, May 14, 2001.
84. "Computational Studies of Transition Metal Biologicals;" NIH, NC-Frederick, ABCC, May 15, 2001.
85. "Modeling Open-Shell Transition Metal Systems;" Southeast Theoretical Chemistry Association, May 18, 2001.
86. "Adventures in Modeling Transition Metals. Challenges, Solutions and Applications;" U of North Texas, Feb. 28, 2002.
87. "Adventures in Modeling Transition Metals. Challenges, Solutions and Applications;" U of South Alabama – March 22, 2002
88. "Adventures in Modeling Transition Metals. Challenges, Solutions and Applications;" IUPUI – April 17, 2002.
89. "Adventures in Modeling Transition Metals. Challenges, Solutions and Applications;" U of Maryland, May 1, 2002.
90. "De Novo Structural Prediction of Transition Metal Complexes;" Am. Chem. Soc. National Mtg in Boston, August 2002.
91. "Adventures in Modeling Transition Metals. Challenges, Solutions and Applications;" Illinois Institute of Technology, September 19, 2002.
92. "Adventures in Modeling Transition Metals. Challenges, Solutions and Applications;" Northwestern State University, January 31, 2003.
93. "Traditional and Nontraditional Modeling of Metal Complexes;" University of Babes-Bolyai University, Cluj, Romania, August 8, 2003.
94. "Modeling of Metal Ions in Chemical and Biological Systems;" Texas Women's University, September 19, 2003.
95. "Modeling of Metal Ions in Chemical and Biological Systems;" UNT Biology Department, November 21, 2003.
96. "Semi-empirical Modeling of Transition Metals;" First Michael Dewar Memorial Symposium at the Anaheim ACS Meeting, March 28-April 1, 2004.
97. "Modeling of Metal Ions in Chemical and Biological Systems;" Tarleton State University, Stephenville, TX, March 24, 2004.
98. "Modeling of Metal Ions in Chemical and Biological Systems;" University of Texas - Brownsville, March 26, 2004.
99. "Modeling of Metal Ions in Chemical and Biological Systems;" University of Oklahoma, April 12, 2004.
100. "Modeling of Metal Ions in Chemical and Biological Systems;" Oklahoma State University, April 13, 2004.
101. "Modeling of Metal Ions in Chemical and Biological Systems;" UNT, Department of Physics, September 21, 2004.
102. "Adventures in Modeling Transition Metals. Challenges, Solutions and Applications;" Loyola University, November 15, 2004.
103. "Modeling Metals in Chemistry and Biology;" East Central University (OK), September 30, 2005.
104. "Modeling Metals in Chemistry and Biology;" Southern Methodist University, February 24, 2006.
105. "Modeling Metals in Chemistry and Biology;" Indiana University, September 8, 2006.
106. "Modeling Metals in Chemistry and Biology;" University of Texas – San Antonio, October 6, 2006.
107. "Modeling Metals in Chemistry and Biology;" Tulane University, November 27, 2006.
108. "Modeling Metals in Chemistry and Biology;" UNT Health Sciences Center, Department of Pharmacology and Neuroscience, February 6, 2007.
109. "Modeling of Metals in Biology. The Role of Electronic Spin in Metal Chemistry;" Steven F. Austin State University, March 22, 2007.
110. "Fun With Metals: Modeling the Catalytic Chemistry of Transition Metals;" Austin Peay State University, April 13, 2007.
111. "Fun With Metals: Modeling the Catalytic Chemistry of Transition Metals;" Southeastern Louisiana University, April 20, 2007.

112. “Modeling of Metals in Biology. The Role of Electronic Spin in Metal Chemistry;" Georgetown University, April 27, 2007.
113. “Modeling of Metals in Chemistry and Biology;" West Texas A&M University, October 5, 2007.
114. “Modeling of Metals in Chemistry and Biology;" LeTourneau University, January 17, 2008.
115. “Modeling of Metals in Chemistry and Biology;" University of North Texas, Materials Science and Engineering, March 7, 2008.
116. “Modeling of Metals in Chemistry and Biology;" New Mexico State University, March 21, 2008.
117. “Rational Design of Transition Metal Catalysts – Past, Current and Future Perspectives;” DOE Catalysis Conference National Meeting, May 2008.
118. “Rational Design of Transition Metal Catalysts – Past, Current and Future Perspectives;” ACS National Meeting, Philadelphia, PA, August 2008.
119. "Rational Design of Organometallic Catalysts;" Gordon Conference on Organometallic Chemistry, Salve Regina U., Newport, R. I., July 2009.
120. *"Pd-Catalyzed Amination;" Southwest Theoretical Chemistry Association Meeting, Houston, October 17, 2009.*
121. "Fun with Metals in Chemistry, Biology and Material Science;" Exxon R&D, Baytown-Texas, October 23, 2009.
122. "Fun with Metals in Chemistry, Biology and Material Science;" Emory University, February 9, 2010.
123. "Fun with Metals in Chemistry, Biology and Material Science;" University of Texas - Arlington, February 19, 2010.
124. "Fun with Metals in Chemistry, Biology and Material Science;" Texas Christian University, February 23, 2010.
125. "Fun with Metals in Chemistry, Biology and Material Science;" Texas Lutheran University, February 26, 2010.
126. "Modeling of Transition Metal Chemistry in Catalysis and Material Science;" Eastman Chemical, Longview, Texas, April 23, 2010.
127. “Further Down the Road to Computer-Aided Catalyst Design;” University of Florida, Department of Chemistry, September 27, 2010.
128. “A Computational Chemist’s Adventures in the Material Science Wonderland;” University of Florida, Department of Material Science, September 29, 2010.
129. “Modeling of Transition Metals in Catalysis and Material Science;” University of South Florida, September 30, 2010.
130. “Modeling of Transition Metals in Catalysis and Material Science;” University of Missouri - Columbia, October 8, 2010.
131. “Further Down the Road to Computer-Aided Catalyst Design;” University of Memphis, Department of Chemistry, October 29, 2010.
132. “Molecular Theory for Real Systems and Chemical Reactions: Chemical Reactions of Complex System with Heavy Elements;” Pacifichem 2010, December 2010, Honolulu.
133. “Securing Our Energy Future through Computational Chemistry!” University of Chicago, Department of Chemistry, January 28, 2011.
134. “The Peter (Wolczanski) Principles: Can They Teach Us Anything About Catalysis?” 241st ACS National Meeting, Wolczanski Award Symposium, March 27, 2011.
135. “Catalyst Design: What Can We Learn from Enzymes and Biological Modeling?” 16th International Workshop on Quantum Systems in Chemistry and Physics (QSCP-XVI), Kanazawa, Japan, September 11-17, 2011.
136. “Catalyst Design: Can We Learn Anything from Enzymes and Biological Modeling?” Argonne National Lab, Chemical Sciences and Engineering, October 11, 2011.
137. “Spin States and Transition Metal Catalyst Modeling;” Mesilla Chemistry Workshop, Las Cruces, NM, February 11 – 15, 2012.
138. “Design of Inorganic and Organometallic Catalysts: Can We Learn Anything from Enzymes and Biological Modeling?” UC-Berkeley, April 13, 2012.
139. “Catalyst Design: What Can We Learn from Enzymes and Biological Modeling?” 16th Theory and Applications of Computational Chemistry (TACC 2012), Pavia, Italy, September 2-7, 2012.
140. **“**Methane to Methanol Catalysis - Integrated Experiment and Modeling Studies in the Center for Catalytic Hydrocarbon Functionalization;” Southwest Regional ACS Meeting, Baton Rouge, LA, Nov 4 – 7, 2012.
141. **“**The Biochemistry of Glutathione, It’s Relationship to Disease and a Century Old Mystery;” Southeast Oklahoma State University, Durant, OK, Nov 15, 2012.

142. "Modeling of Carbon-Hydrogen Bond Activation by Precious and Base Metal Complexes;" Symposium on Organometallic C-H Bond Activation, 245th ACS Annual Meeting, New Orleans, April 9 – 10, 2013.
143. "Computational Adventures In and Around the Oxo Wall;" Hillhouse Award Symposium, 245th ACS Annual Meeting, New Orleans, April 9 – 10, 2013.
144. "Computer-aided Catalyst Design: Or, Can a Blind Squirrel Find a Nut?" Doherty Award Lecture, DFW-ACS Section, September, 2013.
145. "Computer-aided Catalyst Design: Or, Can a Blind Squirrel Find a Nut?" Wichita State University, April, 2014.
146. "Redox Non-innocence of Ligands: Assigning Guilt via Quantum Chemistry;" "Electronic Structure Contributions to Physical Properties and Reactivity in Transition Metal Chemistry" 248th ACS Annual Meeting, San Francisco, August 10 – 14, 2014.
147. "Metal-Methyl + Dioxygen = Fire + Water?;" Hydrogen Peroxide and Dioxygen in Transition Metal Mediated C-H Functionalization Chemistry, 248th ACS Annual Meeting, San Francisco, August 10 – 14, 2014.
148. "Metal-Methyl + Dioxygen = Fire + Water? Catalysts for Selective Oxidation of Methane" UT-Dallas, Sept. 19, 2014.
149. "Metal-Methyl + Dioxygen = Fire + Water? Catalysts for Selective Oxidation of Methane" NCSU, Oct. 17, 2014.
150. **"**Methane to Methanol Catalysis - Integrated Experiment and Modeling Studies;" Duquesne U., Feb 20, 2015.
151. "Ligand Design. Or, Using Computational Chemistry to Help A Blind Squirrel to Find an Acorn;" Gordon Conference on Organometallic Chemistry, Salve Regina U., Newport, R. I., July 2015.
152. "Small But Not So Innocent, The Redox Non-Innocence of Multiply Bonded Ligands. Implications for Catalysis;" Hillhouse Memorial Symposium, 245th ACS Annual Meeting, Boston, August 15 – 19, 2015.
153. "Metal-Methyl + Dioxygen = Fire + Water? Catalysts for Selective Oxidation of Methane" U. Colorado - Denver, Sept. 2015.
154. Controlling the Redox Non-Innocence of Ligands. Implications for Catalysis;" 56th Sanibel Symposium, St. Simon, Georgia, March 13 – 10, 2016.
155. "Modeling The Controlled Burning of Organometallics;" Symposium on Organometallic C-H Bond Activation, Karen Goldberg Symposium, 251st ACS Annual Meeting, San Diego, March 13 – 10, 2016.
156. "Catalysis in the 21st Century: What Role Can/Will Modeling Play?;" ExxonMobil, Baytown, TX, Feb. 2017.
157. "The Aldehyde Water Shift Reaction;" Texas A&M International U., May, 2017.
158. "Small Ligands Behaving Badly: Redox Non-Innocence in Multiply Bonded 3d Metal Complexes;" DOE Contractors Meeting, Gaithersburg, Md., July 2017.
159. "The Aldehyde Water Shift Reaction;" CENTC Symposium on Organometallic C-H Bond Activation, Karen Goldberg Symposium, 253rd ACS Annual Meeting, San Diego, August, 2017.
160. "Catalysis in the 21st Century: What Role Can/Will Modeling Play?;" Southern Methodist University, Dallas, TX, October 2017.
161. "Small Ligands Behaving Badly: Redox Non-Innocence in Multiply Bonded 3d Metal Complexes;" U. Pennsylvania, July 2017.
162. "The Aldehyde Water Shift Reaction;" Pace U. (NYC), November, 2017.
163. "The Biochemistry of Glutathione, It's Relationship to Disease and a Century Old Mystery;" UT – Rio Grande Valley, Edinburg, TX, Feb. 9, 2018.
164. "Modeling Redox Non-Innocence in 3d Metal Complexes;" Symposium on Modeling in Catalysis, 255th ACS Annual Meeting, New Orleans, March 2018.
165. "Modeling Redox Non-Innocence in 3d Metal Complexes;" Computational Chemistry Gordon Conference, July 2018.
166. "Modeling Redox Non-Innocence in 3d Metal Complexes;" U. of Toledo, September 2018.
167. "New Solutions for an Old Problem: Methane Activation;" Inorganic Reaction Mechanisms Gordon Conference, March 2019.
168. "New Solutions for an Old Problem: Methane Activation;" U. Nevada – Reno, Sept. 2019.
169. "New Solutions for an Old Problem: Methane Activation;" ACS Regional Meeting (El Paso), Nov. 2019.
170. "New Solutions for an Old Problem: Methane Activation;" Texas Tech. U., April 2020, via Zoom.
171. "Acid-Base Chemistry of Methane with neither Superacids nor Superbases. A Computational Chemist's Perspective;" Global Inorganic Discussion Weekdays, Chemical Institute of Canada, July 20, 2020, via Zoom.
172. "New Solutions for an Old Problem: Methane Activation;" U. of Memphis, April 2021, via Zoom.

173. “Metal Oxynitride Catalyzed Nitrogen Reduction Reaction;” ACS Annual Meeting, San Diego, March 2022.
174. “Metal Oxynitride Catalyzed Nitrogen Reduction Reaction;” Massasuchetts College of Liberal Arts, Feb. 2023, via Teams.
175. “Metal Oxynitride Catalyzed Nitrogen Reduction Reaction;” Oklahoma U., Chemical Engineering, April 2023.
176. “Metal Oxynitride Catalyzed Nitrogen Reduction Reaction;” UNC Greensboro, April 2023.
177. “Metal Oxynitride Catalyzed Nitrogen Reduction Reaction;” U. Missouri, May 2023.

References

- Mark S. Gordon, Iowa State University, Ames, Iowa 50011: mark@si.msg.chem.iastate.edu
- Peter T. Wolczanski, Cornell University, Ithaca, NY 14853: ptw2@cornell.edu
- Angela K. Wilson, Michigan State University: akwilson@msu.edu

Collaborators, Past and Present

- James Mayer (U Washington), Pete Wolczanski (Cornell), Patrick Holland (UofRochester),
- T. Brent Gunnoe (UVa), Mohammad Omary (UNT), H. V. Rasika Dias (UT-Arlington),
- Mary Anderson (TWU), Angela Wilson (UNT), Tim Warren (Georgetown), Jincheng Du (UNT),
- Srinivasan Srivilliputhur (UNT), Gregory Hillhouse (U. Chicago), Jay Groves (Princeton U.)

Grant History

1. "Computational Investigations of Transition Metal Oxo and Imido Complexes: Important Catalytic and Biochemical Intermediates;" Memphis State University, Faculty Research Grant 1991, $3,000.
2. "Multiconfiguration Self Consistent Field Studies of Transition Metal Complexes;" National Science Foundation, National Center for Supercomputing Applications 1992, 5 hours of Cray Y-MP supercomputer time.
3. "Computational Chemistry across the Periodic Table: The Lanthanides;" National Science Foundation, San Diego Supercomputer Center, 1992, 20 hours of Cray Y-MP supercomputer time.
4. "Effective Core Potentials for the Lanthanides;" National Institutes of Standards and Technology, Intergovernmental Personnel Assignment, 1992, Summer Visiting Scientist Position, ≈ $7,500.
5. "Computational Studies of Transition Metal Mediated Methane Activation;" National Science Foundation, National Center for Supercomputing Applications 1992, 95 hours of Cray Y-MP supercomputer time.
6. "Computational Chemistry across the Periodic Table: Low-, Medium- and High-valent Lanthanide and Transition Metal Complexes;" National Science Foundation, San Diego Supercomputer Center, 1992, 37 hours of Cray Y-MP supercomputer time.
7. "Computational Studies Relevant to the Chemical Vapor Deposition of Transition Metal-containing Materials;" Air Force Office of Sponsored Research, 1992, $12,000.
8. "Exploiting the Synergism Between Theory and Experiment in Lanthanide Chemistry;" Memphis State University, Faculty Research Grant 1992, $2,996.
9. "C-H Activation by Zr-Imido Complexes: A Parallel Supercomputing, Effective Core Potential Study;" National Science Foundation, Cornell National Supercomputer Facility, Strategic Resources Program, 1993, 5,000 hours of SCRS parallel supercomputer time.
10. "Transition Metal Oxo Complexes: Effective Core Potentials and the iPSC/860;"National Science Foundation, San Diego Supercomputer Center, 1992, 3600 hours of iPSC/860 and Paragon parallel supercomputer time.
11. "C-H Activation by Zr-Imido Complexes: A Parallel Supercomputing, Effective Core Potential Study;" National Science Foundation, Cornell National Supercomputer Facility, Strategic Resources Program,1993, unlimited early access to KSR-1 supercomputer ..
12. "C-H Activation by Zr-Imido Complexes: A Parallel Supercomputing, Effective Core Potential Study;" National Science Foundation, Cornell National Supercomputer Facility, Strategic Resources Program, 1993 - 1994 , unlimited early access to SP-1 parallel supercomputer .
13. Department of Energy, Oak Ridge National Labs/University of Tennessee Knoxville; Joint Institute for Computational Science;" 1992 - , unlimited access to iPSC/860 parallel supercomputer.
14. Department of Energy, Oak Ridge National Labs/University of Tennessee Knoxville; Joint Institute for Computational Science;" 1993 - , unlimited access to CM-5 parallel Supercomputer.
15. Air Force Office of Scientific Research, Summer Faculty Research Program, Edwards Air Force Base, 1993, $7,500.

16. "Computational Studies of Lanthanide Chemistry," International Business Machines, Academic Developer's Grant and Joint Study Agreement, 1992 - 1993, equipment discounts totaling ≈ $21,000.
17. "Computational Studies of Transition Metal-Mediated Methane Activation;" American Chemical Society, Petroleum Research Fund, 1993 - 1995, $20,000.
18. "Towards Computer-Aided Catalyst Design: Five Effective Core Potential Studies of Methane Activation;" National Science Foundation, 1994 - 1996, $120,000.
19. "Methane Activation by Multiply-Bonded Transition Metal Complexes - A Vector/Parallel Metacomputing Study;" National Science Foundation, National Center for Supercomputing Applications, 1994, 95 hours of Cray Y-MP; 1000 hours of CM-5 supercomputer time.
20. "Transition Metal Chalcogenido Complexes: A Parallel-Vector Study of Increasingly Realistic Models;" National Science Foundation, San Diego Supercomputer Center, 1994 - 1995, 50 hours of Cray Y-MP supercomputer time and 3600 hours of Paragon supercomputer time.
21. "Towards Computer-Aided Catalyst Design: Three Effective Core Potential Studies of Methane Activation;" Department of Energy, 1994 - 1996, $93,186.
22. "Computational Studies Relevant to the Chemical Vapor Deposition of Transition Metal-containing Materials;" Air Force Office of Sponsored Research, 1994 - 1996, $13,000.
23. "Methane Activation by Multiply-Bonded Transition Metal Complexes;" National Science Foundation, Cornell Theory Center, 1994 - 1995, 2000 hours of KSR-1 supercomputer time.
24. "Effective Core Potential Studies of Bond Activation and Chemical Vapor Deposition Pathways;" National Science Foundation, Cornell Theory Center, 1994 - 1995, 5000 hours of SP-1 supercomputer time.
25. "Towards Computer-aided Design of Metallodrugs. Platinum Antitumor Agents;" National Institutes of Health, Frederick Biomedical Supercomputing Center, 1995 - 1996, 10 hours of computing time.
26. "Towards Computer-aided Design of Metallodrugs. Platinum Antitumor Agents;" University of Memphis, Faculty Research Grant, 1995, $3,994.
27. "Methane Activation by Mercury(II) Complexes;" National Science Foundation, Research Experiences for Undergraduates, 1996, $4,000.
28. "Methane Activation by Mercury(II) Complexes;" American Chemical Society, Petroleum Research Foundation, 1996, $47,000.
29. "Renovation of J. M. Smith Chemistry Building at University of Memphis;" National Science Foundation, Academic Research Infrastructure, $294,422 (including $188,431 UM matching), 1996.
30. "Studies of Medium-Valent Complexes: Methane Activation and Anticancer Drugs;" National Science Foundation, Cornell Theory Center, 1996, 4000 hours of SP2 supercomputer time.
31. "Solvent Effects in Methane Activation by Mercury Complexes;" American Chemical Society, Petroleum Research Foundation, 1996, $5,000. Summer Supplement for stay of visiting professor Dr. Kimberly Lawler (Cal State - Fresno).
32. "Computational Studies of Transition Metal Bonding and Reactivity;" National Science Foundation, 1997 - 1999, $180,000.
33. "Accurate Quantum Calculation of Nonlinear Optical Properties for Transition Metal Complexes;" National Science Foundation, National Center for Supercomputing Applications, 4000 SUs on SGI Power Challenge (collaboration with Prof. Henry Kurtz).
34. "Dynamics of Advanced Material Precursor Decomposition. A Computational Study;" National Science Foundation, Cornell Theory Center, 1997, 5000 hours of SP2 supercomputer time.
35. "Acquisition of a Computational Chemistry Resource for the University of Memphis," National Science Foundation, 1997, $290,717 (including $105,359 UM match).
36. "Towards Computer-aided Design of Lanthanide Complexes," Travel Grant to attend 5th Chemical Congress of North America, American Chemical Society and National Science Foundation, 1997, $500.
37. "Bonding Structure and Reactivity of Multiply Bonded Complexes;" Department of Energy, 1997 - 2000, $171,000.
38. "Theory-Experiment Study of Transition Metal/C-H Bond Interactions;" National Science Foundation, International Programs, 1998 - 1999, $4,880.
39. "NLO Properties of Transition Metal Complexes;" National Center for Supercomputing Applications, 40,000 SUs on SGI Power Challenge (collaboration with Prof. Henry Kurtz).
40. "Carbon-Hydrogen Bond Activation by Ti-Imidos;" National Science Foundation, San Diego Supercomputer Center, 4,000 SUs on IBM SP-2, 1998 - 1999.
41. “Effective Core Potential Methods in Hartree-Fock and Density Functional Theory;” ACS-PRF, Type SE Grant, $2,000. 1999 – 2000.
42. "Improved Modeling Techniques for Metal-based Biologicals;" National Science Foundation Scholar in Residence at NIH, $43,700, 2000 - 2001.

43. "Computational Studies of Inorganic and Organometallic Complexes;" National Science Foundation, $170,000, 2000 - 2003.
44. "A Summer at the Interface between Theory and Experiment;" National Science Foundation - Research Experiences for Undergraduates, $98,073, 2000 - 2003.
45. "Improved Modeling of Transition Metal Materials - Applications to Catalysis and Technetium Chemistry;" DOE, $230,000, 2000 - 2004.
46. "Soft Computing Modeling of Catalysis. US-Romanian International Collaboration;" NSF, International Programs, $44,641, 2000 – 2003.
47. "Genetic Algorithm Solution of the Schrodinger Wave Equation;" NCSA, NT SuperCluster, 10,000 SUs, 2000 – 2001.
48. "Novel Approaches to Quantum Modeling of Chemical Systems. US-Indian International Collaboration;" NSF, International Programs, $25,000, 2001 – 2004.
49. "Research Experiences for Undergraduates in Chemistry at the University of North Texas;" co-PI with Prof. Angela K. Wilson, $161,061, 2003- 2006.
50. "Purchase of a Computing Cluster for UNT Chemistry;" National Science Foundation, co-PI with Profs. Angela K. Wilson, Paul Marshall, Paul Bagus, Marty Schwartz, and Mohammad Omary, $129,484, 2004-2007.
51. "Regional Center for Advanced Scientific Computing and Modeling;" Department of Education, co-PI with Prof. Angela K. Wilson, $248,000, 2005 – 2008.
52. "Computational Studies of Ligand and Catalyst Design and Catalytic Mechanisms;" Department of Energy, 2005 - 2008, $255,000.
53. "Research Experiences for Undergraduates in Chemistry at the University of North Texas;" co-PI with Prof. Angela K. Wilson, $172,000, 2007- 2010.
54. "Structure and Reactivity of Low Coordination Transition Metal Complexes;" National Science Foundation, PI, $270,000, 2007 – 2011.
55. "Institute for Science and Engineering Simulation: Aircraft Fatigue Modeling and Simulation;" Air Force Research Laboratory (WPAFB), co-PI with Profs. Angela Wilson, Alan Needleman (UNT MS&E), Raj Banerjee (UNT MS&E); $9,000,000; 2008 – 2011.
56. "Acquisition of a Computational Resource for the Department of Chemistry at the University of North Texas;" National Science Foundation, Co-PI with Angela Wilson and Mike Richmond, $360,139, 2008 – 2011.
57. "Metal-Organic Field Effect Transistors (MOFETs);" co-PI with Profs. Mohammad A. Omary (UNT) and Bruce Gnade (UT-Dallas); Norman Hackerman Advanced Research Program (NHARP) awards, Advanced Research Program (ARP) and the Advanced Technology Program (ATP), Texas Higher Education Coordinating Board, $150,000 (UNT portion is $93,000); 2008-2010.
58. "Modeling of Catalytic Processes for More Efficient Utilization of Hydrocarbon Resources;" Department of Energy, Basic Energy Sciences, 2008 – 2011, $300,000.
59. "Environmental and Energy Research at the Texas Center for Advanced Scientific Computing and Modeling (CASCaM);" co-PI with Prof. Angela K. Wilson, Department of Energy, Biological and Environmental Research, 2008 – 2015, $1,417,304.
60. "Center for Catalytic Hydrocarbon Functionalization;" Energy Frontier Research Centers, PI: T. Brent Gunnoe (UVa), Co-PI. 2009 – 2015, $1,000,000 (UNT portion).
61. "Metalloaromatic Multinuclear Complexes of Monovalent Coinage Metals: Novel Chemistry Driving Applications in Molecular Electronics;" co-PI with Profs. Mohammad A. Omary (UNT), Jincheng Du (UNT), and Bruce Gnade (UT-Dallas); NSF-CRC, $1,300,000 2009-2012.
62. "Center for Enabling New Technologies Through Catalysis (CENTC);" PI: Karen I. Goldberg with 16 Senior Investigators at 14 institutions; NSF-CCI; sub-contract from the University of Washington; Total Award Amount: $15,456,971 (UNT portion $257,598); 01/01/2011 - 07/31/2017.
63. "Modeling of Late Transition Metal Catalysts for Energy Applications;" DOE-BES (PI); $324,000; 9/15/2011 - 09/14/2016.
64. "Modeling of Catalytic Bond Functionalization by Base and Noble Metal Catalysts;" NSF-CHE (PI); $330,000; 9/15/2011 - 09/14/2015.
65. "Earth-abundant Metal Catalysts for the Functionalization of Strong Carbon-Hydrogen Bonds;" CHE-1464943, NSF-CHE, $361,927, 2015 – 2018.
66. "MRI: Acquisition of a Computer Cluster for the Computational Chemistry Program at the University of North Texas, CHE-1531468, 2015 – 2018.
67. "Modeling of Catalytic Processes for More Efficient Utilization of Hydrocarbon Resources;" DOE-BES (PI); $324,000; 8/14/2016 - 8/14/2019, $362,465.

68. "Activation of Light Alkanes by Earth-abundant Metal-Oxo Complexes;" ACS-PRF (PI); $110,000; 8/14/2016 - 8/14/2018.
69. "Hydridic Methane Activation;" Welch Foundation (PI, co-PI with M. Anderson (TWU)); $195,000; 6/1/19 – 5/31/22.
70. "Modeling of Biological Systems;" Reata Pharmaceuticals; 9/16/2011 - 4/15/2021, ~ $135K per annum (co-PI with A. Wilson, MSU).
71. "Fundamental Acid/Base Properties of Hydrocarbon C-H Bonds and Metal-Elements Active Sites;" NSF-CHE, 2020 – 2023, $376K
72. "Metal Oxynitrides: Tuning Metal-N and Metal-O Interactions for Improved Electrocatalytic Properties at the Liquid/Solid Interface;" NSF-DMR, 2021 – 2024, (co-PI with J. Kelber and F. D'Souza), $500K
73. "MRI: Acquisition of a High Performance Hybrid Computer Cluster for Computational Modeling;" NSF-OAC, 2021 – 2024, $686K.
74. "Development of Novel Approaches to Earth-abundant Methane Catalysis;" DOE-BES, $247K

Graduate Students and Postdoctoral Researchers

1. Eddie W. Moody (MS: Fall 92 - Summer 94; Ph.D. Fall 94 - Spring 97)
Ph. D. Dissertation: "Artificial Intelligence Applications in Inorganic Chemistry" (**1997**)
M. S. Thesis: "Towards the Computer Aided Design of Magnetic Resonance Imaging Contrast Agents: A Molecular Mechanics Force Field for Gd Complexes" (**1994**)

2. Yueping Li (MS: Fall 92 - Summer 94)
Project(s): Modeling of CVD Reactions
M. S. Thesis: Effective Core Potential Modeling of Group IVA-Group IVB Chemical Vapor Deposition (**1994**).

3. Phil Raby (MS: Spring 94 - Summer 96)
M. S. Thesis: An Effective Core Potential Study of Transition Metal-Chalcogenidos. Vibrational Analysis (**1996**).

4. Michael T. Benson (Ph.D.: Summer 93 - Summer 97)
Ph. D. Dissertation: Computational Studies of Late Transition Metal Complexes and Experimental Studies of Lanthanide Coordination Complexes (**1997**).

5. Akihiko Yoshikawa (Ph.D. Fall 94 - Summer 98)
Ph. D. Dissertation: Methane Activation by Mercury Complexes (**1998**).

6. Wentao Fu (Ph. D. Fall 95 - Summer 99)
Ph.D. Dissertation: Computational Studies of Transition Metal Pharmaceuticals and Advanced Materials (**1999**)

7. Tie Zhou (Ph.D. Summer 96 - Spring 00)
Ph.D. Dissertation: Modeling Nonlinear Optical Properties of Inorganic Complexes (**2000**).

8. Jun Deng (Ph.D.: Summer 97 – Summer 2001)
Ph.D. Dissertation: Development and Application of Traditional and Non-traditional Modeling Methods for Transition Metal Chemistry (**2001**).

9. Tom Klinckman (Ph.D.: Summer 97 – Spring 01)
Ph.D. Dissertation: C-H Activation by High and Low Valent Transition Metal Complexes (**2001**).

10. Yong Zhao (Ph.D.: Summer 99 – Summer 2003)
Ph.D. Dissertation: Computational Study of Carbon-carbon and Carbon-Heteroatom Bond Formation (**2003**).

11. Dr. Steve Decker (NSERC Postdoc: Jan 2000 – June 2001)
Project(s): ECP/DFT Studies of NO Scission and Aqueous-phase Hydroformylation

12. Christopher Taylor (MS: Van Vleet & Hackett Fellow, Summer 00 – Summer 02)
Masters Thesis: Olefin Insertion and Subsequent B-X Elimination from a Pentacoordinated Tantalum Complex. A Density Functional Theory Study (**2002**).

13. Karl Pittard (MS: Summer 00 – Summer 02)
Masters Thesis: A Synthetic and Computational Approach to Ligand Design and Electronic Studies of Fluorinated Phosphine Chelates (**2002**).

14. Corneliu Buda (PhD: Fall 00 – Fall 04)
PhD Dissertation: De novo prediction of the ground state structure of transition metal complexes (**2005**).

15. Adriana Dinescu (MS: Fall 02 – Spring 04)
(PhD: Spring 04 – Spring 2007)
Masters Thesis: Modeling Wild Type and Mutant Glutathione Synthetase (**2004**).
PhD Dissertation: Metals in Chemistry. Computational Chemistry Studies (**2007**).

16. Khaldoon Barakat (MS: Fall 02 – Spring 04)
(PhD: Spring 04 – Fall 07)
Masters Thesis: Modeling the Chemical and Photophysical Properties of Gold Complexes (**2004**).
PhD Dissertation: Computation Studies of Selected Ruthenium Catalysis Reactions (**2007**).

17. Sridhar Vaddadi (PhD: Fall 02 – Fall 06)
PhD Dissertation: Computational Studies of Coordinatively Unsaturated Transition Metal Complexes (**2006**).

18. Eduard Baba (MS: Fall 02 – Fall 04)
Master's Thesis: N-Heterocyclic Carbenes of the Late Transition Metals: A Computational and Structural Database Study (**2004**)

19. Tom Grimes (PhD: Fall 04 – Fall 07)
PhD Dissertation: Quantum Perspectives on Physical and Inorganic Chemistry (**2007**).

20. Dr. Nathan J. DeYonker (PostDoc: Spring '05 – Spring '09)
Project(s): Composite Methods for Accurate Main Group and Transition Metal Thermodynamics

21. Samer Tekarli (PhD: Fall 05 – Spring 11)
PhD Dissertation: Computational Investigation of Molecular Optoelectronic and Biological Systems (**2011**).

22. Aaron Pierpont (PhD: Fall 06 – Summer 10)
PhD Dissertation: Computational Study of Small Molecule Activation via Low-Coordinate Late First-Row Transition Metal Complexes (**2010**).

23. Glenn Morello (PhD: Fall 07 – Summer 11)
PhD Dissertation: Modeling Transition Metal Chemistry for Catalytic Functionalization of Molecules (**2011**).

24. H. Emanuel Gonzalez (PhD: Summer 08 – Fall 2012)
Project(s): Pt-catalyzed C-H Bond Activation, CO_2-"omics"
PhD Dissertation: Group 10 Catalyzed Olefin Hydroarylation (**2012**).

25. Bhaskar Chilukuri (PhD: Fall 08 – Summer 12)
PhD Dissertation: Rational Design of Metal-Organic Electronic Devices: A Computational Perspective (**2012**).

26. Dr. Jamal Uddin (PostDoc: Fall 09 – Fall 10)
Project(s): Composite Methods for Accurate Main Group and Transition Metal Thermodynamics

27. Dr. Mike Drummond (Research Associate: Fall 09 – Fall 12)
Project(s): Composite Methods for Accurate Main Group and Transition Metal Thermodynamics

28. Olayinka Olatunji-Ojo (PhD: Summer 09 – Summer 13)
Project(s): Meso- and Multi-scale Modeling of CO_2 Fluidics, NILs

29. Bruce Prince (PhD: Fall 09 – Fall 13)
Project(s): Pt-NHC Chemistry, Oxy-insertion, C-H Activation

30. Travis Figg (PhD: Fall 09 – Spring 13)
Project(s): Orgaonmetallic Baeyer-Villiger Reactions

31. Dr. Jason McAfee (PostDoc: Spring 10 – Spring 11)
Project(s): Multiscale Modeling of Methane Functionalization

32. Daniel Pardue (PhD: Fall 10 – Summer 15)
Project(s): Oxy-Insertion and C-H Bond Activation by Earth Abundant Metals

33. Dale Pahls (PhD: Summer 11 – Spring 15)
Project(s): Rh-Catalyzed C-O Bond Formation, O_2 Chemistry of Organometallics

34. Dr. Claire McMullin (PostDoc: Summer 11 – Fall 12)
Project(s): Late Transition Metal Catalysis

35. Brandall Ingle (PhD: Fall 11 – Spring 15)
Project(s): Negative Cooperativity in Human Glutathione Synthetase, Peptide Bond Formation

36. Dr. George Schoendorff (PostDoc: Spring 12 – Spring 16)
Project(s): Lanthanide Chemistry

37. Hengameh Fallah (PhD: Fall 13 – Spring 17)
Project(s): Reductive C—X Bond Functionalization

38. Sarah Khani (MS: Spring 14 – Spring 16)
Project(s): "Oid" Chemistry, Hydroarylation Catalysis

39. Quan Jiang (PhD: Spring 14 – Fall 2018)
Project(s): Pd Amination, Co-mediate C-F Bond Activation

40. Yavuz Ceylan (PhD: Fall 15 – Spring 2019)
Project(s): Pd Catalyzed Styrene Synthesis, Boride Complexes

41. Riffat Parveen (PhD: Spring 16 – Spring 2019)
Project(s): Ta and Re Mediated Methane Activation, Ancillary Ligand Effects, Ni ARD, Polymerization

42. Daniel Zhicheng Sun (PhD: Fall 16 – Fall 20)
Project(s): Activation of Methane by PDI Complexes, Catalysis for Organic Synthetic Transformations

43. Azadeh Nazemi (PhD: Fall 16 – Spring 20)
Project(s): pKa of C-H Bonds, PCET

44. Ahmad Najafian (PhD: Fall 16 – Spring 20)
Project(s): Methane Activation by Transition Metal Methoxides, Ammonia Electro-oxidation

45. Catherine Moulder (PhD: Fall 17 – Spring 21)
Project(s): Transition metal thermochemistry, NSF Graduate Fellow

46. Carly Carter (PhD: Fall 18 – Spring 2022)
Project(s): Main group-based methane activators, olefin polymerization

47. William Grumbles (PhD: Fall 18 – Summer 2022)
Project(s): pKa of metal-methyl complexes

48. Kortney Melancon (PhD: Fall 19 – Fall 20)
Project(s): Benzoin condensation catalyzed by NHCs

49. Megan Ericson (MS: Fall 19 – Spring 20)
Project(s): Coinage metal chemistry

50. Domllermut Alamo Velazquez (PhD: Fall 19 – Fall 2022)
Project(s): Nitridyl C—H activation

51. Colton Lund (PhD: Fall 19 – present)
Project(s): Azide decomposition

52. Ignacio Migliaro (PhD: Spring 20 – present)
Project(s): Methane activation by frustrated Lewis pairs

53. Waad Alharbi (PhD: Spring 20 – Summer 23)
Project(s): Nitride activation of C-H Bonds, Basicity of Nitrides

54. Mojgan Gharaee (PhD: Spring 20 – present)
Project(s): Ti- and Co- Alloyed Nitrides, Co-oxynitride NRR catalysis

55. Seyed Alireza Hajiseyed Javadi (PhD: Spring 22 – present)
Project(s): Porphyrin based NRR

56. Cooper Kimbrough (PhD: Spring 20 – present)
Project(s): CMD

Other Graduate Students Who Have Done Research in the Cundari Lab

1.	Lynn Strohecker	Ln & TM Computations
2.	George Richardson	Methane Activation by $W(OH)_2(NH)_2$
3.	Chryssanthi Stylianopoulos	Modeling of Vanadium Complexes
4.	James Morse	Modeling of CVD
5.	Alex Gonser	Gold Chemistry
6.	Stacy Payne	DFTB Studies of CO_2 Sequestration
7.	E. Chauncey Garrett	Oxy-insertion as a Function of d-Count

Graduate Student/Postdoctoral "Sabbaticals"

1.	Mike Benson	U. of Windsor (Doug Stephan)	Organometallic Synthesis

*MT Benson, DW Stephan, Niobium and Tantalum Diphosphanato Complexes: Synthesis, Structure, and NMR Studies of $Cp_2MH[(PR)_2]$ (R = Ph, Cy, H) Organometallics **1997**; 16; 3504 - 3510.*

2.	Wentao Fu	U. of Florida (Mike Zerner)	Lanthanide Semiempirical Calculations
3.	Tie Zhou	IUPUI (Cliff Dykstra)	Modeling NLO Properties

*T Zhou, CE Dykstra Additivity and Transferability of Atomic Contributions to Molecular Second Dipole Hyperpolarizabilities J. Phys. Chem. A **2000**, 104, 2204 - 2210.*

4.	Tom Klinckman	Los Alamos (Jeff Hay)	Actinide Modeling
5.	Steve Decker	Iowa State U. (Mark Gordon)	Modeling Solvation Effects
6.	Tom Grimes	Osaka Prefecture University (NSF EAPSI Fellow)	Modeling Spin-Orbit Effects
7.	Aaron Pierpoint	National University of Singapore (NSF EAPSI Fellow)	Solid State Modeling
8.	Bhaskar Chilukuri	North Carolina St. U. (M. Whangbo)	Solid State Modeling

		Ga. Tech (J-L. Bredas)	ET at MOFET Interfaces
9.	Hengameh Fallah	UNC-Chapel Hill (AJ Miller)	Hydricity

Undergraduate Students

	Student	**Dates**	**Research**
1.	Soon J. Lim	(1992)	Metal-Oxos
2.	Stacy Toney	(1992)	Metal-Oxos
3.	Timara Faulkner	(1992)	Metal-Oxos
4.	Karen Pierce-Beaver	(1993)	Metal-Sulfidos
5.	Jefferey A. Wiggins	(1993)	Metal-Sulfidos
6.	M. Leigh Lutz (PSU-Erie)	(1993 - 4)	Methane Activation by Group IIIA Methyls
7.	Hoang D. Nguyen	(1993 - 4)	Metal-Sulfidos
8.	Lynn Tippett	(1993 - 4)	II/VI & Lanthanide Complexes
9.	Giao T. Le	(1994)	II/VI Compounds
10.	Scot A. Curtiss	(1995)	Vib Spectra of Metal-Chalcogenidos
11.	Debra Smith	(1995)	Vib Spectra of Metal-Chalcogenidos
12.	Enrique Ignarra (Barry U)	(1994 - 5)	Lanthanide Complexes
13.	Ikea T. Mallory	(1995)	Platinum Complexes
14.	Jason Maté (Barry U)	(1995)	Platinum Complexes
15.	Leigh Anne Snyder	(1995 - 6)	Pt Drugs & Hg Catalysts
16.	Chryssanthi Stylianopoulos	(1996)	Vanadium Complexes
17.	Leah C. Saunders	(1996 - 8)	Anti-AIDS & Gd Drugs
18.	Laura L. Sisterhen	(1996 - 7)	Vanadium Complexes
19.	Tom R. Klinckman (APSU)	(1995 - 6)	Pt(II) & Pt(IV) Complexes
20.	Mary V. Cocke	(1997 - 8)	Chromium Complexes
21.	Melissa Beaugrand	(1997)	Technetium Complexes
22.	James C. Ham	(1997)	AI applications in IC
23.	Sharon Maclin	(1998)	UV-vis spectra of metallates
24.	Julie Kemker	(1998)	Chromium Complexes
25.	Chris Morris (USA)	(1998 - 2000)	Rhodium Vaska Complexes
26.	David Ball	(2001 - 2)	Tc Complexes
27.	Aaron Gillespie (UNCW)	(2001)	Tc Complexes
28.	Danielle Temple (Lyon)	(2002)	Ligand Design
29.	Aubri Waters	(2003)	TM Thermochemistry
30.	Denise Parker	(2003)	TM Thermochemistry
31.	Justin Lee	(2004)	Copper Catalysis
32.	Lloyd Spaine (McNair Fellow)	(2005-8)	Copper Catalysis
33.	Dustin Ho	(2005-7)	TM Thermochemistry
34.	David Melton	(2007-8)	A_{2a} Adenosine Receptor
35.	Karthik Janani	(2007-8)	Imidene Chemistry
36.	Soheil Gharahi	(2007-8)	Imidene Chemistry
37.	Matt Amme	(2007-8)	Copper Catalysis
38.	Johnny Vo	(2007-8)	Imidene Chemistry
39.	Jordan Braunfeld	(2008-10)	CO_2 & Biocatalysis
40.	Smitha Janardan	(2008-10)	First Principles Modeling of NiAl
41.	Rebeca Lopez	(2009)	Allosteric Pathways in hGS
42.	Daisy Hao	(2009)	NiC Interatomic Potentials
43.	Tim Wu	(2010)	SCA Analysis of hGS
44.	Brooke Otten	(2009-12)	Oxygen Atom Transfer
45.	Kurtis Carsch	(2009-12)	C-H Activation by Low Valent Metal-Oxos
46.	Ryan Bartling	(2010)	Analytical EAM Models
47.	David Chi	(2010)	C-H Activation by Low Valent Metal-Oxos
48.	Cody Freitag	(2011-13)	Alkoxide/Amide Metathesis
49.	William Ou	(2012-14)	Alkoxide/Amide Metathesis
50.	Shannon Teaw	(2013-14)	Reductive Functionalization with Co Complexes
51.	Franklin Jia	(2013-15)	Reductive Functionalization with Co Complexes
52.	Brittany Thornton	(2013-15)	Reductive Functionalization with Co Complexes
53.	Justin Qian	(2013-15)	Reductive Functionalization with Co Complexes

54.	Carolyn Guan	(2014-6)	Aziridination by 3d Nitrenes and Nitrenoids
55.	Floyd Horng	(2014-6)	Reductive Func. With Earth Abundant Grp 6 Metals
56.	Catherine Moulder	(2015-7)	Methane Activation by Metal Imide Complexes
57.	Franklin Zhang	(2015-6)	Ethylbenzene Dehydrogenase Mimics
58.	Aakash Sambhariya	(2015-6)	Ethylbenzene Dehydrogenase Mimics
59.	Andy Wu	(2016-6)	Methoxide Complexes
60.	Eduardo Montoya	(2016-8)	Ancillary Ligand Effects
61.	Elaine Lee	(2016-7)	Organometallic pKa's
62.	Garren Ferreira	(2017-9)	Organometallic pKa's
63.	Christopher Zhou	(2018 -	Organometallic pKa's & machine learning
64.	Amy Guan	(2019 -	Methane activation as a function of pKa(C—H)
65.	Ivy Liang	(2019 -	Methane activation as a function of pKa(C—H)
66.	Drishti Gupta	(2021 -	Methane activation by main group compounds
67.	Nathan Beard	(2022 -	Basicity of dinitrogen complexes

Student Fellowships and Awards

1.	Mike Benson	1996 - 1997	Van Vleet Fellowship (UM)
2.	Mike Benson	1994	Los Alamos Graduate Research Assistantship
3.	Tom Klinckman	1999	Los Alamos Seaborg Fellowship
4.	Jun Deng	2000 - 2001	University of Memphis Society Fellowship
5.	Tom Klinckman	2000	DOE Student Travel Fellowship, Annual Meeting of Nobel Laureates in Lindau, Germany
6.	Steve Decker	2000 - 2002	NSERC (Canada) Postdoctoral Fellowship
7.	Christopher Taylor	2000 - 2004	Van Vleet Fellowship
8.	Christopher Taylor	2000 - 2003	Hackett Fellowship
9.	Jun Deng	2001	Women's Research Forum: Outstanding Female Graduate Award (1st recipient)
10.	Adriana Dinescu	2004	George Vaughan Memorial Award
		2007	James J. and Ruth I. Spurlock Award
		2007	Graduate Council Dissertation Award
11.	Tom Grimes	2004 - 2005	Toulouse First-Year Doctoral Fellowship
		2006	George Vaughan Memorial Award
		2007	Ed and Julia Hodges Memorial Scholarship
12.	Aaron Pierpont	2006 - 2007	Toulouse First-Year Doctoral Fellowship
		2006	George Vaughan Memorial Award
		2010	James J. and Ruth I. Spurlock Award
13.	Glenn Morello	2008 - 2009	CAS Graduate Research Fellowship
2009		George Vaughan Memorial Award	
		2011	James J. and Ruth I. Spurlock Award
14.	Bhaskar Chilukuri	2010	George Vaughan Memorial Award
15.	Travis Figg	2011	George Vaughan Memorial Award
15.	Dale Pahls	2013	George Vaughan Memorial Award
		2014	Ed and Julia Hodges Memorial Scholarship

NSF Research Experience for Undergraduate (REU) Students

1.	Leigh-Anne Snyder (UofM)	Summer 1996	Methane Activation by Hg Complexes
2.	Misha Golynskiy (Truman)	Summer 2000	Synthesis of Novel Phosphines (w/ RG Peters)
3.	Jacob Reichman (Drew)	Summer 2000	Synthesis of Novel Phosphines (w/ RG Peters)
4.	Scott Cook (Southern Nazarene)	Summer 2000	Photochromic Organometallics (w/ TJ Burkey)
5.	Brian Holmes (UofM)	Summer 2000	Photochromic Organometallics (w/ TJ Burkey)
6.	Tom Louis (Centenary)	Summer 2001	Novels Phosphines for Hydroformylation (w/ RGP)
7.	KD Cooney (Carroll College)	Summer 2002	Phosphite Ligand Design (w/ RGP)
8.	Ian Firkin (James Madison)	Summer 2002	N-Heterocyclic Carbenes
9.	Alondra Flores (UT-Brownsville)	Summer 2003	Coordination Isomerism
10.	Tom Grimes (LeTourneau)	Summer 2003	Thermochemistry
11.	Clinton Whitely (Benedictine)	Summer 2004	Oxygen Atom Transfer
12.	Aaron Pierpont (Central CT)	Summer 2005	Carbon-Hydrogen Bond Activation

13.	Rachel Combs (Rice U)	Summer 2005	Phosphorus-Carbon Bond Cleavage
14.	Sara Hernandez (TWU)	Summer 2007	Glutathione Synthetase
15.	Chauncey Garrett (MC)	Summer 2007	Thermochemistry of Cyclohexadienyl Radical
16.	Margie DeJesus (TWU)	Summer 2008	CO_2 "omics"
17.	Vanessa Johnson (TWU)	Summer 2008	CO_2 "omics"
18.	Nelli Bodiford (UTA)	Summer 2009	Carbothermal Synthesis
19.	Francisco Birk (UF)	Summer 2011	Amide/Alkoxide Metathesis
20.	Austin Green (PSU)	Summer 2013	$PdO + H_2$ Potential Energy Surface
21.	Theresa Warner (Miami U., Ohio)	Summer 2014	Catalyst Regeneration with O_2 and Acid
22.	Andrea Marton (UF)	Summer 2014	Nature and Reactivity of γ-Mo_2N Surfaces
23.	Robert Adams (CSU-DH)	Summer 2015	Calculation of Redox Potentials
24.	Antonio Lopez (St. Mary's)	Summer 2015	Calculation of Redox Potentials
25.	Jacob Williams (U. Wyo.)	Summer 2016	Oxidation of Iridium Hydride Complexes
26.	Olivia Hull (Wichita St. U.)	Summer 2016	Methane Activation by Nitride Complexes
27.	Kent Lopez (NIU)	Summer 2017	Redox Innocent Complexes
28.	Max Mrozek-McCourt (Monmouth)	Summer 2019	Co-oxynitride modeling

Visiting Faculty Members and Scientists

1.	Prof. Kimberly Lawler	Cal-State Fresno ('97)	Solvent Effects in Methane Activation
2.	Prof. Shaun Sommerer	Barry U ('97)	Multiply Bonded Complexes
3.	Prof. Norris Hoffman	U. South Alabama ('00)	Rh-Vaska Complexes
4.	Jorge Juan Carbo	UA Barcelona ('00)	QM/MM Studies of Hydroformylation
5.	Prof. Dave White	UNC-Wilmington ('01)	*De Novo* Prediction of TM Geometry
6.	Prof. Costel Sarbu	Babes-Bolyai U ('01,'02)	AI Modeling of Metal Catalysis
7.	Prof. Horia Pop	Babes-Bolyai U ('01,'02)	AI Modeling of Metal Catalysis
8.	Rajendra Saha	IACS ('02)	AI Solutions of the SWE
9.	Prof. Abul Kazi	UA-Pine Bluff ('03-'05)	Linkage Isomerism
10.	Dr. Gideon Steyl	U. Free State (SoAf, '03,'05)	TM Thermochemistry
11.	Prof. Hassan Rabaâ	Ibn Tofail U (Morocco, '04,'05)	CH Activation
12.	J. Oscar Jiminez-Halla	U Girona ('06)	Catalysis
13.	Sarah Barelier	INSA-Lyon ('07)	Modeling of Human Glutathione Synthetase
14.	Prof. Art Low	Tarleton State U. ('07)	Solid State Calculations of MOFs
15.	Zhuofeng Ke	Sun-Yat Sen U. ('07-'08)	Amination of Benzene
16.	Matt Remy	U of Michigan/CENTC ('08)	Pd Catalysis
17.	J. Brannon Gary	U of Michigan/CENTC ('08)	Pd Catalysis
18.	Dale Pahls	UIUC/CENTC ('09)	ELF Calculations of Catalysts
19.	Ting Li	UR/CENTC ('09)	Ni-Allyl Catalysis Modeling
20.	James Morris	UofR/CENTC ('09)	Ni-mediated Bond Activation
21.	Prof. Rory Waterman	U. Vermont ('10)	Zr Catalysis Modeling
22.	Karla Erickson	U. Vermont ('10)	Zr Catalysis Modeling
23.	Sarina Bellows	UofR ('11)	$Fe/N_2/H_2$ Chemistry
24.	Amanda Cook	U of Michigan/CENTC ('13)	Pd Acetate Chemistry
25.	Taylor Stevens	UW/CENTC ('15)	N-C Bond Formation
26.	Vitor Hugo Menezes da Silva	U. Sao Paolo	Ni-Catalyzed Heck Reaction
27.	Dr. Glen Alliger	Exxon	Catalysis Modeling
28.	Hannah Zeitler	U. Penn ('20)	Pincer ligands